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A PHYSICAL MODEL FOR COMPUTING FLUID FLOW SOLUTIONS

William P. Wright

September 1977

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USA ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
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A physical and mathematical scheme is described which can be the basis for the construction of a computer program designed to solve fluid flow problems important to the U.S. Army. Essentially the scheme consists of the determination of contributions of moments of physical quantities over Lagrangian cells of fluid, which move according to the local fluid velocity to neighboring fixed cells. Based on the sums of these contributions of moments, new distributions across the fixed cells are determined which correspond to fluid flow

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during an elapse of a finite interval of time. The moments of the physical quantities over subregions of the Lagrangian cells are evaluated by utilizing a set of integral equations which are derived in the report.

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I. INTRODUCTION

Fragment penetration of fuel cells is a traditional damage and kill mechanism of the Army's motorized vehicles and fuel storage containers. In order to provide information which will assist in understanding the physical phenomena involved, it was decided that a new approach for simulating fluid flow may be of value. Consequently, a completely general formulation was conceived to serve as the basis for the development of a computer code.[1]

The purpose of this report is to document the basic ideas given in the original notes and to present an expansion of them in a form suitable for use as a guide in the construction of a code. It is not the intention of this report to discuss all of the physics which would be involved in such an undertaking. Presented here is a mathematical description of the procedure for simulating fluid flow by combining Lagrangian cell motion and the computation of distributions of physical quantities over cells based on a knowledge of moments over subregions of the cell.

II. THE BASIS OF THE PROPOSED NUMERICAL TECHNIQUE FOR TRANSPORTING PHYSICAL QUANTITIES IN FLUID FLOW

The numerical technique for simulating fluid flow transport consists of two separate parts; the sum of which will yield distributions of the physical parameters across fixed cells as a function of time. While the discussion is presented in terms of rectilinear coordinates, the same theory is applicable in cylindrical or spherical coordinates and, in fact, the code should be constructed to accomodate all three. To facilitate understanding, the discussion will concentrate on one part of the numerical technique at a time.

Figure II-1 consists of a diagram which portrays cells assumed to be formed by a fixed rectangular coordinate system x, y. The two dimensional assumption implied by the figure is not necessary since the arguments are equally valid in one, two, or three dimensions. In each cell an arbitrary physical parameter is represented by the symbol α_J. The subscript J is to denote that the distribution of α corresponding to each J cell, can be different. This situation is assumed to exist at time t_s, which would be the instant corresponding to that at the beginning of a cycle of computation.

In each of the four cells depicted in Figure II-1, the fluid has associated with it a local velocity distribution of the form presented in Figure II-2. As indicated, the two components, $\vec{v}_x$ and $\vec{v}_y$, are assumed

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[1] *Rogers, Joel, unpublished progress reports submitted to the Ballistic Research Laboratory, March 9, 1970 and January 19, 1971.*

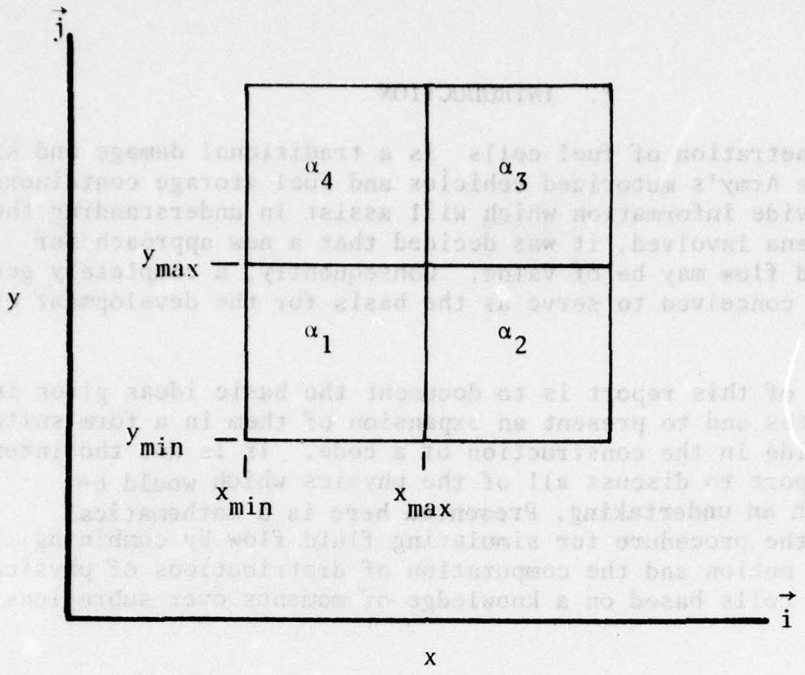

Figure II-1 Cell Representation In Fixed Coordinates at t_s.

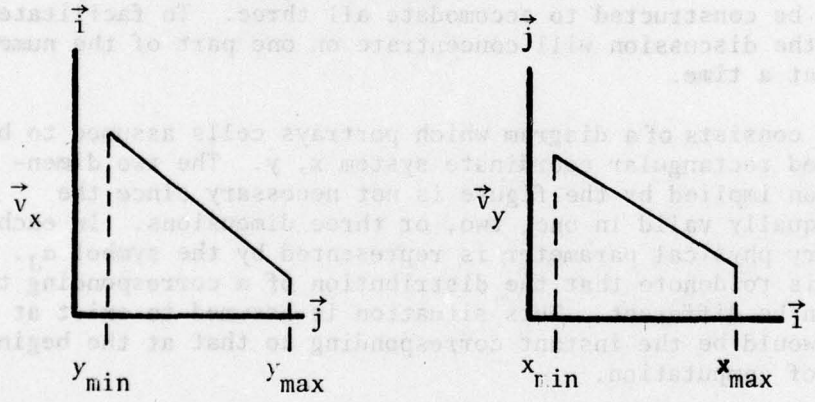

Figure II-2 Local Fluid Velocity Distribution.

to be linear and in general are represented by the following expressions:

$$\vec{v}_x = \vec{i}\,(a_1\, y + a_2)$$
$$\vec{v}_y = \vec{j}\,(a_3\, x + a_4) \qquad \text{(II-1)}$$

where $\vec{i}$ and $\vec{j}$ are unit directional vectors and a_1, a_2, a_3, and a_4 are coefficients.

Treating the fluid in the cells of Figure II-1 as Lagrangian cells which move as bodies of fluid according to the fluid's local velocity, the new positions of these Lagrangian cells at $t_s + \Delta t$ can be obtained and are represented by the dashed lines in Figure II-3. The symbol Δt represents a finite interval of time. The shaded regions, denoted by SR_J, constitute contributions of the moments of physical parameters from the four Lagrangian cells to one cell in the fixed coordinate system. The immediate task is to explain how to obtain the distributions of the physical parameters based on these four contributions.

The basis for the procedure for computing the distribution of the physical parameter is presented in Appendix A. There is shown that if certain moments of the physical parameter are available for the subregions, then a new distribution based on these moments can be calculated for that parameter across the total region. To accomplish this, it is necessary to resolve the question as to which moments are required and how are the moments obtained? For the present, we may hold the latter portion of the question in abeyance and assume that the moments are available. The decision, relative to the first part of the question above, depends on the form of the distribution of the physical parameter desired as we will demonstrate by the following example.

First of all, we may arbitrarily assume that the distribution of the physical parameter α, in Figure II-3, is to be of a linear form as follows:

$$\alpha = b_1 x + b_2 y + b_3 \qquad \text{(II-2)}$$

where α is a function of the spatial parameters x and y and b_1, b_2, and b_3 are coefficients to be evaluated.* In order to evaluate the three coefficients, it is sufficient to generate three equations containing these coefficients and to solve them simultaneously. To this end, we multiply through Equation II-2 by a function f which is required to

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**The linear assumption assumed here is not necessary in that a higher order polynomial may be utilized. In any case the same procedure is to be followed.*

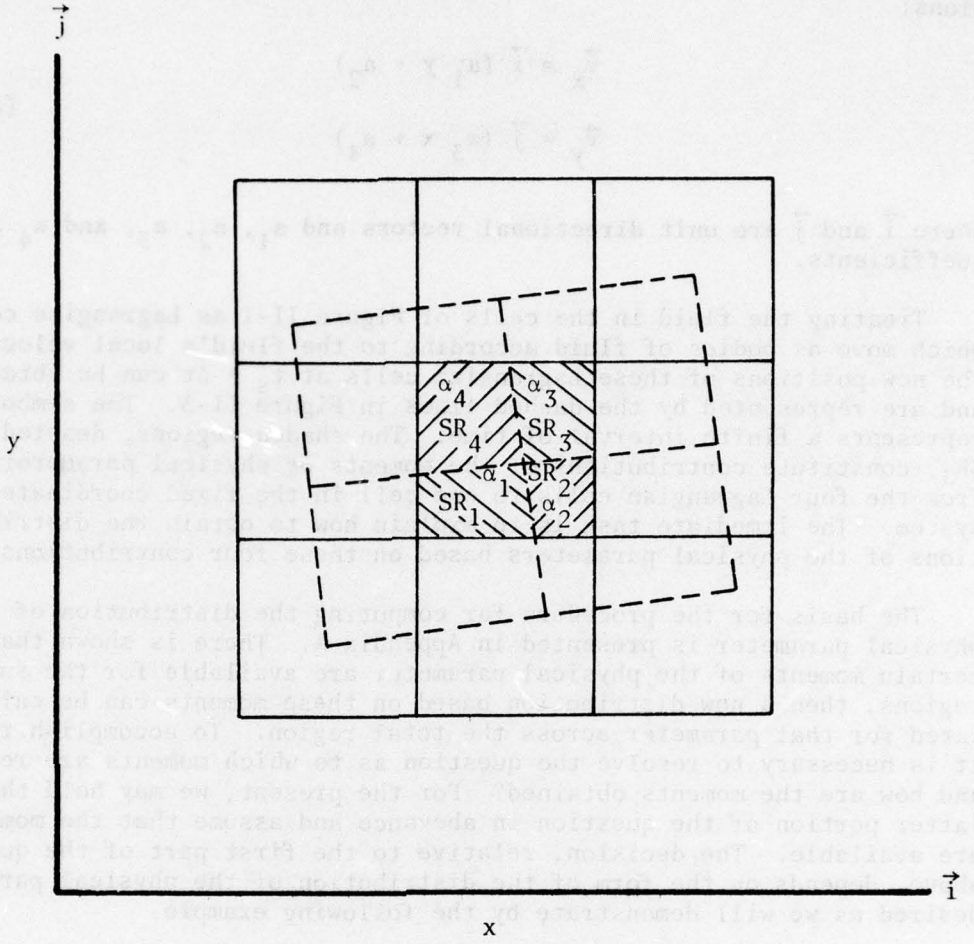


Figure II-3 Contributions Of Moments Of A Physical Parameter To Fixed Cell At $t_s + \Delta t$.

take on values of 1, x, and y. That is:

$$f\,\alpha = b_1\, f\,x + b_2\, f\,y + b_3 \tag{II-3}$$

and

$$\begin{aligned} \alpha &= b_1\, x + b_2\, y + b_3 \\ x\,\alpha &= b_1\, x^2 + b_2\, x\, y + b_3\, x \\ y\,\alpha &= b_1\, x\, y + b_2\, y^2 + b_3\, y\ . \end{aligned} \tag{II-4}$$

Integrating the terms of Equations II-4 with respect to x and y yields the following equations:

$$\begin{aligned} \int_{TC} \alpha\, dA &= b_1 \int_{TC} x\, dA + b_2 \int_{TC} y\, dA + b_3 \int_{TC} dA \\ \int_{TC} x\,\alpha\, dA &= b_1 \int_{TC} x^2\, dA + b_2 \int_{TC} x\, y\, dA + b_3 \int_{TC} x\, dA \\ \int_{TC} y\,\alpha\, dA &= b_1 \int_{TC} x\, y\, dA + b_2 \int_{TC} y^2\, dA + b_3 \int_{TC} y\, dA \end{aligned} \tag{II-5}$$

where dA equals dx dy and the symbol TC is intended to indicate that the integrations are to be performed over limits which span the entire cell (from x_{min} and y_{min} to x_{max} and y_{max} respectively in Figure II-1). For other forms of the distribution, the function f would be set equal to other values, but in general:

$$f = x^{k_1}\, y^{k_2} \tag{II-6}$$

where k_1 and k_2 are equal to 0, 1, 2, ... For combinations of these values for k_1 and k_2, the values of f are 1, x, y, x y, x^2y, xy^2, x^2y^2, and etc.*

The integrals on the right side of Equations II-5 depend on the limits defined by the coordinate values of the corner points of the cell and are easily evaluated. We refer to them as Geometric Moments because their values depend on the spatial parameters only, and for convenience,

The proposed distributions for density, momentum, and kinetic energy and the required moments are presented in detail in Appendix C.

we represent them by the symbol G as follows:

$$G_1 = \int_{TC} dA$$

$$G_2 = \int_{TC} y \, dA$$

$$G_3 = \int_{TC} x \, dA \qquad \text{(II-7)}$$

$$G_4 = \int_{TC} xy \, dA$$

$$G_5 = \int_{TC} x^2 \, dA$$

$$G_6 = \int_{TC} x^2 \, dA \; .$$

Substitution of Equations II-7 into Equations II-5 yields the following equations:

$$\int_{TC} \alpha \, dA = b_1 G_3 + b_2 G_2 + b_3 G_1$$

$$\int_{TC} x \, \alpha \, dA = b_1 G_5 + b_2 G_4 + b_3 G_3 \qquad \text{(II-8)}$$

$$\int_{TC} y \, \alpha \, dA = b_1 G_4 + b_2 G_6 + b_3 G_2 \; .$$

The integrals on the left are equal to the sums of the integrals over the various subregions. Consequently, the following equations can be written:

$$\int_{TC} \alpha \, dA = \int_{SR_1} \alpha_1 \, dA + \int_{SR_2} \alpha_2 \, dA + \int_{SR_3} \alpha_3 \, dA + \int_{SR_4} \alpha_4 \, dA$$

$$\int_{TC} x \, \alpha \, dA = \int_{SR_1} x \, \alpha_1 \, dA + \int_{SR_2} x \, \alpha_2 \, dA + \int_{SR_3} x \, \alpha_3 \, dA + \int_{SR_4} x \, \alpha_4 \, dA \qquad \text{(II-9)}$$

$$\int_{TC} y \, \alpha \, dA = \int_{SR_1} y \, \alpha_1 \, dA + \int_{SR_2} y \, \alpha_2 \, dA + \int_{SR_3} y \, \alpha_3 \, dA + \int_{SR_4} y \, \alpha_4 \, dA$$

where SR_J indicates that the limits of integrations extend over the various subregions.

We obtain the following equations after combining Equations II-8 and Equations II-9:

$$\sum_J \int_{SR_J} \alpha_J \, dA = b_1 G_3 + b_2 G_2 + b_3 G_1$$

$$\sum_J \int_{SR_J} x \, \alpha_J \, dA = b_1 G_5 + b_2 G_4 + b_3 G_3 \qquad \text{(II-10)}$$

$$\sum_J \int_{SR_J} y \, \alpha_J \, dA = b_1 G_4 + b_2 G_6 + b_3 G_2 \, .$$

The remaining task consist of evaluating the moments of the physical parameter over the various subregions as indicated by the integrals on the left side of Equations II-10 and the shaded regions in Figure II-3. The limits of these subregions can be determined by the intersections of the boundaries of the Lagrangian cell and the fixed coordinate system's cells. However, the distributions of α_J are unknown since changes in α_J have occurred over the time step Δt, and thus the integrals cannot be evaluated directly.

In Figure II-4A, a Lagrangian cell of fluid is shown at $t_s + \Delta t$, where the subregions are formed by the intersections of the boundaries. Since the motion of the cell is calculated using the local fluid velocity and the time step Δt, the limits of these subregions can be converted by the reverse process to limits of corresponding subregions for the cell located at t_s, as shown in Figure II-4B. The distribution of α is known

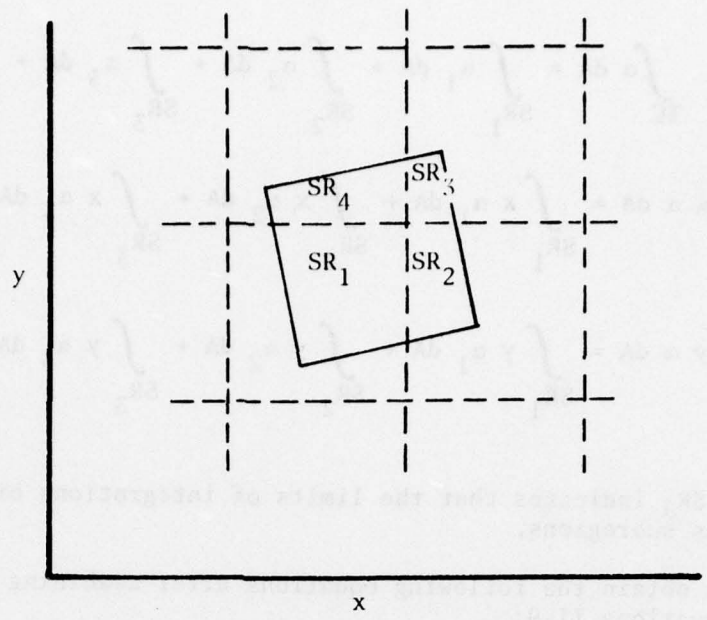


Figure II-4A Lagrangian Cell Position In Fixed Coordinates At $t_s + \Delta t$.

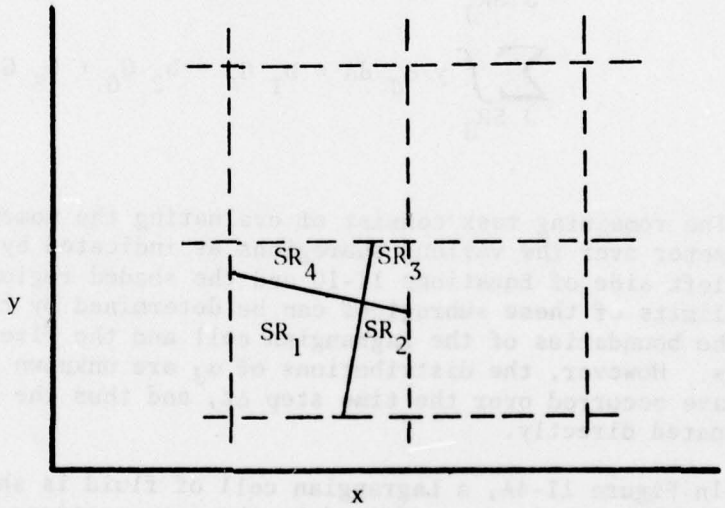


Figure II-4B Lagrangian Cell Position In Fixed Coordinates At t_s.

at t_s, thus if the integrals for calculating moments could be evaluated over the limits at t_s, such that the results are equivalent to those at $t_s + \Delta t$, then the difficulty would be resolved.

In order to permit integrations at t_s, the function $f(x,y,t)$ is defined at $t_s + \Delta t$ as follows:

$$f(x, y, t_s + \Delta t) = x^{k_1} y^{k_2} \qquad \text{(II-11)}$$

and is required to satisfy the following differential equation:

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = 0 \ . \qquad \text{(II-12)}$$

This differential equation is to be interpreted as saying that f is a constant along particle paths. Thus, to first order accuracy, we have

$$f(x, y, t_s) = f\ (x + \vec{v}_x \Delta t, y + \vec{v}_y \Delta t, t_s + \Delta t) \qquad \text{(II-13)}$$

where x, y are the global coordinates of the fixed coordinate system.

In Appendix B, the Equation II-12 and the conservation equations of change are utilized in deriving the appropriate equations of change needed to compute moments of the physical parameters over the subregion at t_s.

III. A COMPUTATIONAL VERIFICATION OF THE METHOD

A satisfactory verification of the method proposed in this report demands a comparison with computations of complicated problems solved with existing codes using already "proven" methods. This is currently impossible since the program, utilizing this proposed method, has not been constructed. Consequently, the best one can do at this point is to solve a simple problem for the purpose of demonstrating that the proposed method for simulating fluid flow is feasible. In addition, such a calculation may be helpful in providing a means whereby the method can be better understood. In any case, this section is intended to verify the method to a limited extent and should be approached from that point of view.

The problem chosen is the determination of the steady velocity distribution for flow between two semi-infinite parallel flat plates, where the driving mechanism is the frictional forces due to the constant

motion of one of the plates. Diagrams, describing the temporal aspect of the problem, are presented in Figure III-1. In the diagram at the top of Figure III-1, the velocity is zero throughout the fluid for times prior to some arbitrary instant of time t_0. At t_0, the lower plate is set in motion suddenly at some velocity (in this case the value 0.8 is assumed) and due to the frictional force between the plate and the fluid, the fluid is dragged along with the plate. It is assumed that no slippage exist between the surfaces of the fluid and the plates; thus that layer of fluid adjacent to the surface of the plates and the plates have the same velocity. For all time after t_0, the lower plate is forced to retain its initial velocity and momentum is continuously transferred in the y direction from the moving plate to the fluid and through the fluid toward the upper plate. The momentum is transferred from one layer of fluid to the next due to the frictional force created by the effect of the viscosity of the fluid. Since the upper plate is forced to remain motionless, the velocity of the layer of fluid adjacent to its surface remains zero. Eventually the steady velocity distribution is obtained, as shown in the bottom diagram of Figure III-1. The objective of the calculation is to determine momentum distributions of the fluid from t_0 until the steady velocity distribution is obtained. It is not necessary to simulate a real fluid to make our point, thus simple values are used for the parameters involved and no reference to specific units are made.

The fluid motion in this flow problem is in one direction only; that being in a direction parallel to the plates. The form of the velocity distribution is written as follows:

$$\vec{v}_x = \vec{i}\,(a_1\, y + a_2) \qquad \text{(III-1)}$$

where

$\vec{v}_x$ = the velocity parallel to the plates.

y = the coordinate perpendicular to the plates in the $\vec{j}$ direction.

$\vec{i}$ = the unit vector in the direction parallel to the plates.

a_1, a_2 - coefficients.

The motion of the Lagrangian cell is demonstrated in Figures III-2 and III-3, where the dashed lines represent the cells formed by the fixed coordinate system and the solid lines indicate the positions of the Lagrangian cells at $t_s + \Delta t$. Focussing attention on the T row of cells in Figure III-2, we see that the cells of fluid are partitioned into two subregions by the intersection of boundaries. The shaded

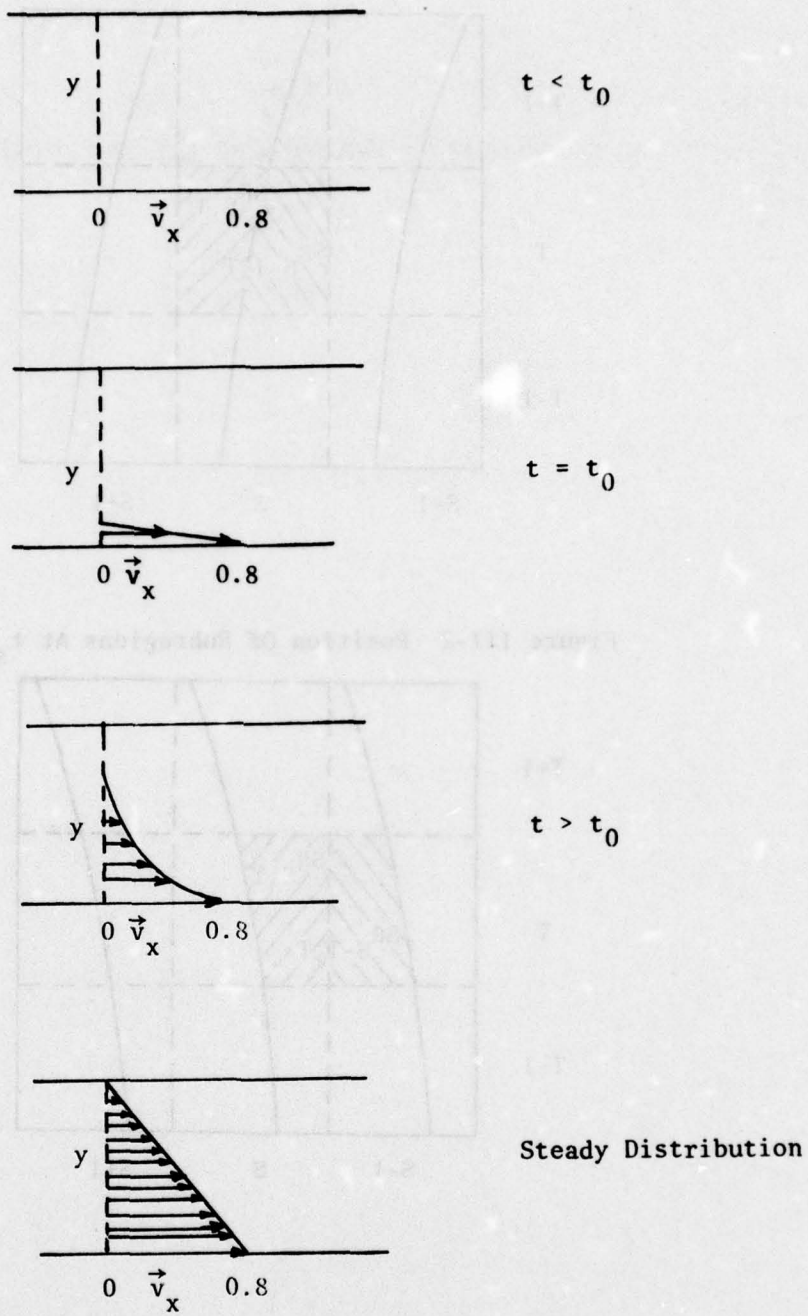


Figure III-1 Velocity Distributions For Fluid Between Semi-infinite Parallel Flat Plates As A Function Of Time.

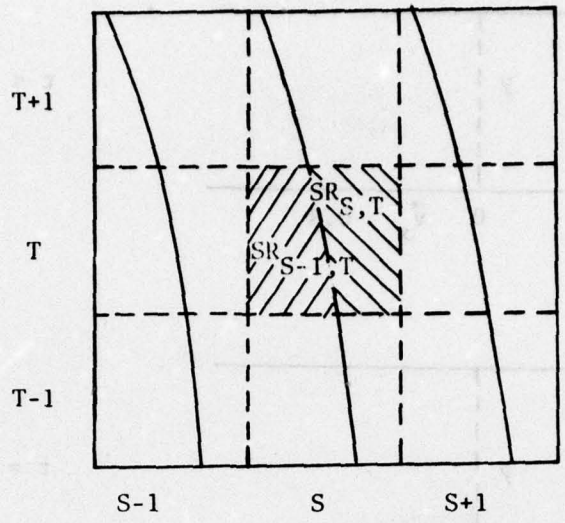


Figure III-2 Position Of Subregions At $t_s + \Delta t$.

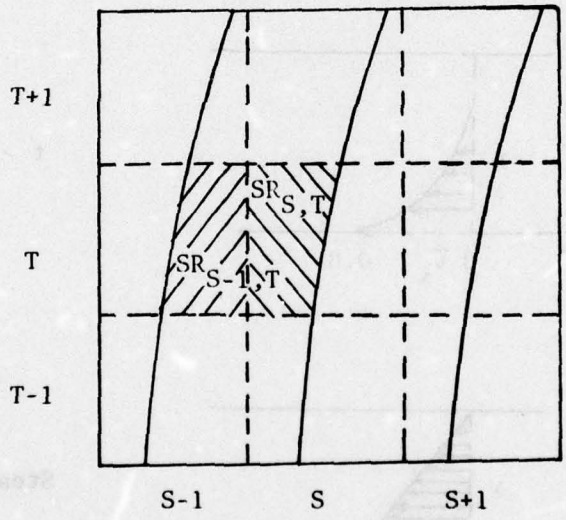


Figure III-3 Position Of Subregions At t_s.

subregions represent the contributions of fluid from Lagrangian cells, which were initially superimposed on (S-1,T) and (S,T) fixed cells at t_s, to the fixed cell (S,T) at $t_s + \Delta t$. Based on this information, the fixed cells, to which the contributions from the various subregions are to be summed, are identified. The motion of the Lagrangian cells are computed by translating the corner points with the Equation III-1 and a time step Δt.

In this problem, at any point in time, the flow does not vary in the $\vec{i}$ direction parallel to the flat plates. Consequently the velocity distribution at $t_s + \Delta t$ need be determined in only one column of cells (say Column S of Figure III-2). However, the procedure required an additional column of cells (Column S-1 in Figure III-2) in order to obtain the contribution of flow from one column of cells into the next column. In this case the contributions are represented by the subregions identified as $SR_{S-1,T}$ and $SR_{S,T}$. At the end of a cycle of computations both columns of cells are given the same velocity distribution as that calculated in order to start the next cycle of computations.

For this problem, only momentum need be considered to obtain the required results. And for simplification, we assume that the density distribution throughout the flow is equal to 1. Therefore, the expression for the momentum is identical to the velocity distribution which is expressed as Equation III-1. Thus, the two moment equations needed to obtain the velocity or momentum distribution across the fixed cell at $t_s + \Delta t$ are written as follows:

$$\int_{SR_{S-1,T}} \vec{v}_x \, dx \, dy + \int_{SR_{S,T}} \vec{v}_x \, dx \, dy = a_1 \int_{TC} y \, dx \, dy + a_2 \int_{TC} dx \, dy \qquad \text{(III-2)}$$

$$\int_{SR_{S-1,T}} y \, \vec{v}_x \, dx \, dy + \int_{SR_{S,T}} \vec{v}_x \, dx \, dy = a_1 \int_{TC} y^2 \, dx \, dy + a_2 \int_{TC} y \, dx \, dy \, .$$

To evaluate the left side of Equations III-2, it is necessary to revert to the subregion's limits at t_s as shown in Figure III-3 and to utilize the integral equation for momentum derived in Appendix B. Since there are no external forces or any imposed pressure gradient, the applicable momentum equations reduce to the following:

$$\int_{SR(t_s+\Delta t)} \rho \vec{v}_x \, dx \, dy = \int_{SR(t_s)} \rho \vec{v}_x \, dx \, dy - \Delta t \int_{SR(t_s)} \vec{\vec{\tau}} \cdot \vec{n} \, dx$$

$$\int_{SR(t_s+\Delta t)} y\rho \vec{v}_x \, dx \, dy = \int_{SR(t_s)} (y + v_y \Delta t) \rho \vec{v}_x \, dx \, dy \qquad \text{(III-3)}$$

$$- \Delta t \int_{SR(t_s)} (y + v_y \Delta t) (\vec{\vec{\tau}} \cdot \vec{n}) \, dx + \Delta t \int_{SR(t_s)} y + v_y \Delta t) \cdot \vec{\vec{\tau}} \, dx \, dy$$

where

$\vec{\vec{\tau}}$ = the stress tensor.

$\vec{n}$ = the unit vector perpendicular to subregion surface as shown in Figure III-4.

$\Delta = \vec{i} \, \partial/\partial x + \vec{j} \, \partial/\partial y$.

ρ = density.

For this problem, the stress tensor reduces to the following:

$$- \mu \left(\vec{i} \, \vec{j} \, \frac{\partial \vec{v}_x}{\partial y} + \vec{j} \, \vec{i} \, \frac{\partial \vec{v}_x}{\partial y} \right) .$$

Consequently, the term

$$\Delta t \int_{SR(t_s)} \Delta y \cdot \vec{\vec{\tau}} \, dx \, dy$$

becomes

$$- \Delta t \int_{SR(t_s)} \mu \frac{\partial v_x}{\partial y} \, dx \, dy \qquad \text{(III-4)}$$

where for simplicitity, the value of the viscosity μ is set equal to 1.

For this two dimensional problem, the second term on the right side of Equation III-3 are line integrals. Since the stress tensor reduces to Equation III-4, the terms in question are, in this case, independent of the y coordinate. Therefore, only integrations along the top and

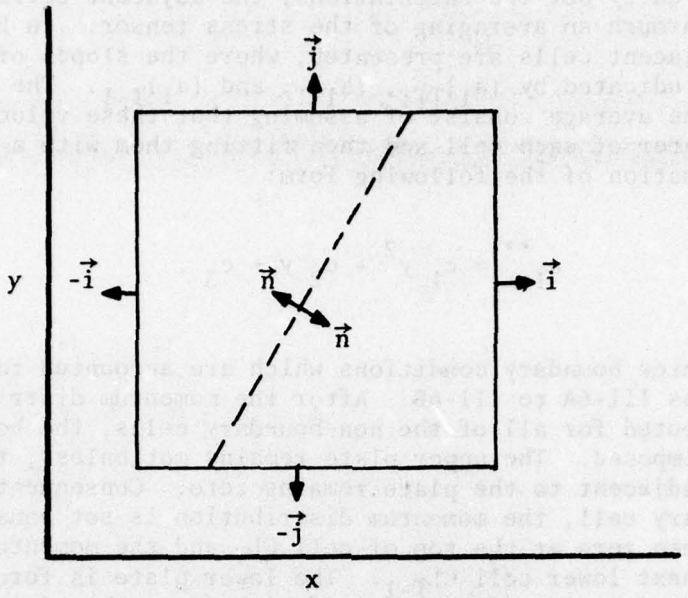


Figure III-4 The Unit Vectors Perpendicular To Surfaces.

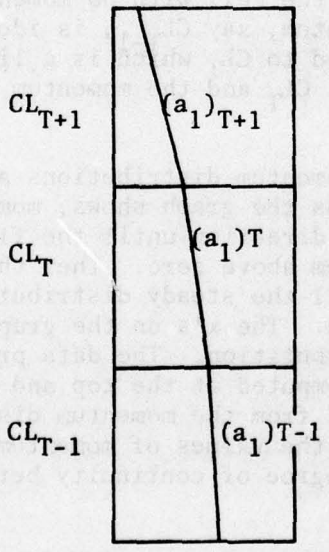


Figure III-5 The Least Square Cubic Fit Of Velocity Slopes.

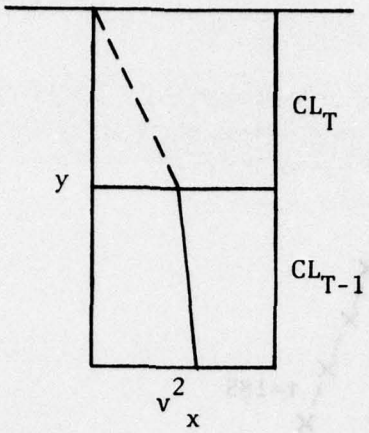
bottom of the subregions are needed.

In order to carry out the calculations, the adjacent cells must be inter-related through an averaging of the stress tensor. In Figure III-5, three adjacent cells are presented, where the slopes of the velocities are indicated by $(a_1)_{T+1}$, $(a_1)_T$, and $(a_1)_{T-1}$. The procedure for obtaining the average consist of assuming that these velocity slopes exist at the center of each cell and then fitting them with a least square cubic equation of the following form:

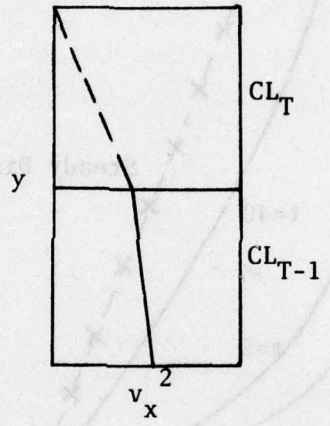
$$a_1^{**} = c_1 y^2 + c_2 y + c_3 . \qquad \text{(III-5)}$$

There are three boundary conditions which are accounted for as diagramed in Figures III-6A to III-6B. After the momentum distribution at $t_s + \Delta t$ is computed for all of the non-boundary cells, the boundary conditions are imposed. The upper plate remains motionless, thus the fluid velocity adjacent to the plate remains zero. Consequently, for the upper boundary cell, the momentum distribution is set equal to a linear fit between zero at the top of cell CL_T and the momentum value at the top of the next lower cell CL_{T-1}. The lower plate is forced to retain a constant velocity of 0.8, thus for the lower boundary cell, the momentum distribution is set equal to a linear fit from the momentum value at the bottom of the next higher cell CL_{T+1} and the constant plate velocity at the bottom of the lower boundary cell CL_T. In addition, as the momentum is propagated in the y direction, there will be some cells with no momentum. Therefore a moving boundary condition exists until all of the cells between the plates have gained some momentum. In order to handle this moving boundary, the cell with no momentum, say CL_T which is adjacent to a cell with momentum, say CL_{T-1}, is identified. Then a momentum distribution is assigned to CL_T which is a linear fit between zero momentum at the top of cell CL_T and the momentum value at the top of cell CL_{T-1}.

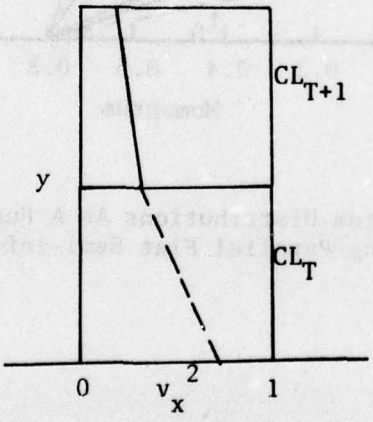
Figure III-7 presents the momentum distributions as a function of y for various instants of time. As the graph shows, momentum was progressively transported in the y direction until the fluid in all of the cells obtained values of momentum above zero. Then the momentum increased in all of the cells until the steady distribution, represented by the dashed line, was obtained. The x's on the graph represent the results of the last cycle of computation. The data presented in Table III-1 represents the momentum computed at the top and bottom of the cells where the values were determined from the momentum distribution. The data indicates the closeness of the values of momentum between adjacent cells and suggests that a high degree of continuity between cells exist using the proposed method.



III-6A Upper Plate Boundary Condition.



III-6B Moving Boundary Condition In Fluid.



III-6C Lower Plate Boundary Condition.

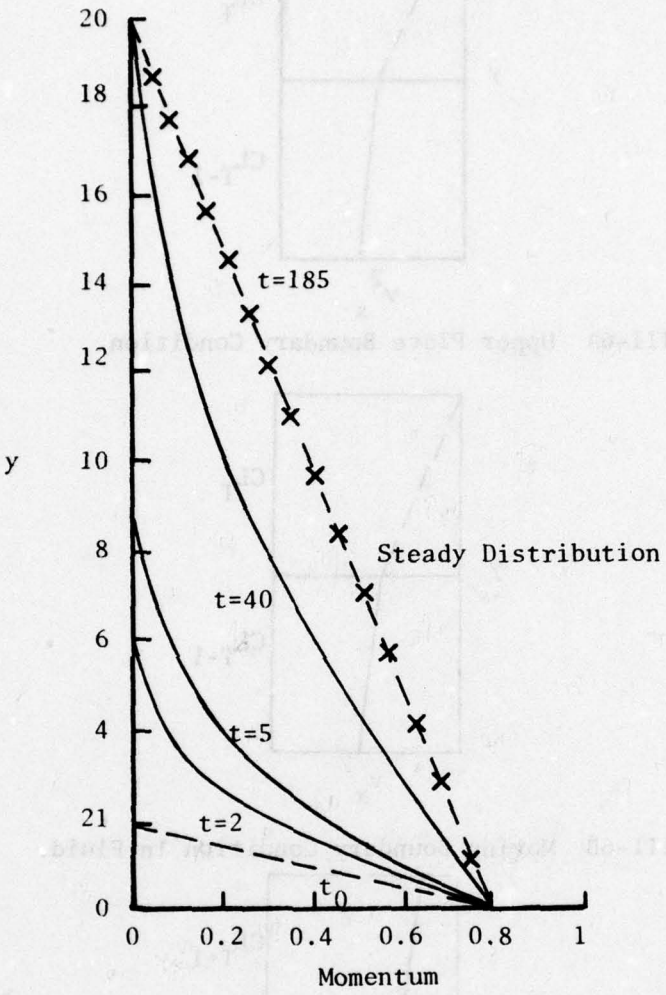


Figure III-7 Momentum Distributions As A Function Of Time For The Sliding Parallel Flat Semi-infinite Plate Problem.

Table III-1. Momentum Values At The Top and Bottom of Cells For The Sliding Plate Problem.*

Cell	Momentum Values	
	Bottom	Top
1	0.8	0.729246870
2	0.729246870	0.659359231
3	0.659359241	0.591170446
4	0.591170426	0.425451446
5	0.525451478	0.462884307
6	0.462884251	0.404040364
7	0.404040364	0.349365223
8	0.349365239	0.299169344
9	0.299169299	0.253625760
10	0.253625788	0.212773912
11	0.212773847	0.176527839
12	0.176527922	0.144689503
13	0.144689462	0.116963056
14	0.116963063	0.092972181
15	0.092972282	0.072275841
16	0.072275821	0.054383357
17	0.054383268	0.038768292
18	0.038768374	0.024879464
19	0.024879485	0.012149046
20	0.012149046	0.0

* $\Delta x = 1$; $\Delta y = 1$; $\Delta time = 0.1$; Time = 40

IV. A CONCEPTUAL DESCRIPTION OF THE CODE CONSTRUCTION

The most efficient device for organizing a conceptual description of a code structure is the flowchart as presented in Figures IV-1 to IV-6. This flowchart is a preliminary effort and is not intended to accomplish more than a demonstration of an overall approach.

That part of the flowchart in Figure IV-1 symbolizes the modeling of a real problem in terms of the actual data required to compute a solution. In general, such a model would be based on the various physical characteristics of the real target and the offensive mechanism with which the target will be engaged. In particular, the geometry of the target, the properties of the materials of which the target is constructed, and any specific initial conditions must be defined. In addition, the offensive mechanism must be characterized and described in an idealized manner appropriate for computer computations. Based on this information, the actual input data for a calculation is to be formalized.

The input model would consist primarily of basic assumptions, boundary conditions, and other basic data associated with the target materials. The basic assumptions deal with items such as the number of dimensions, compressibility, the number of kinds of species, external forces, and etc. The boundary conditions would vary from problem to problem and accounting for them will constitute one of the more difficult tasks. Some of the other basic data referred to above could be vaporization rates, reaction rates, an ignition criteria and etc, which would be needed if the problem required accounting for combustion.

Once the input model has been read into the computer, the code should execute those subroutines designed to compute moments of the physical parameters for all of the cells and then sum them in the appropriate fixed cells. These subroutines are indicated in that part of the flow chart shown in Figures IV-2 and IV-3; beginning at S1 and ending with S3.

Assuming that the cells are numbered consecutively from 1 to a maximum number I_{max}, the code would naturally begin with the I = 1 cell and resolve the question as to whether it is a boundary cell. If the cell is one defining a boundary, the code would activate that subroutine (not shown on the flowchart) which accounts for the appropriate boundary condition corresponding to that cell, and then proceed to the next I cell.

Whenever the cell does not constitute one defining a boundary condition, the code would execute a subroutine entitled "Neighboring Cells" in the flowchart. This subroutine would identify those cells which are adjacent to the current I cell by their I number and these numbers would be stored for future use. The reason this information will be needed is that the Lagrangian cell will deposit its "contents" in certain ones of these neighboring cells, depending on the direction of the fluid velocity.

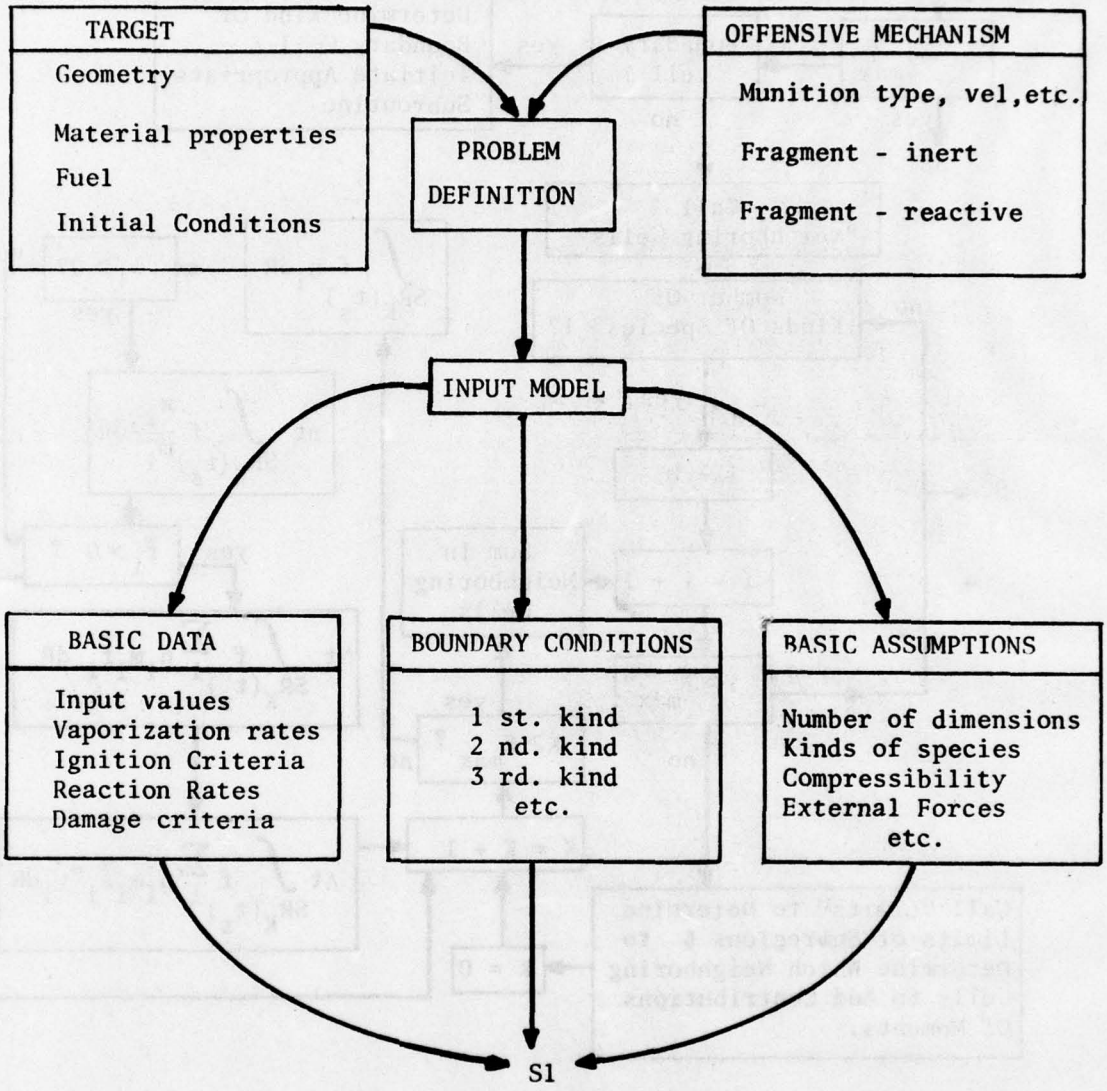


Figure IV-1 Flowchart For Code Construction.

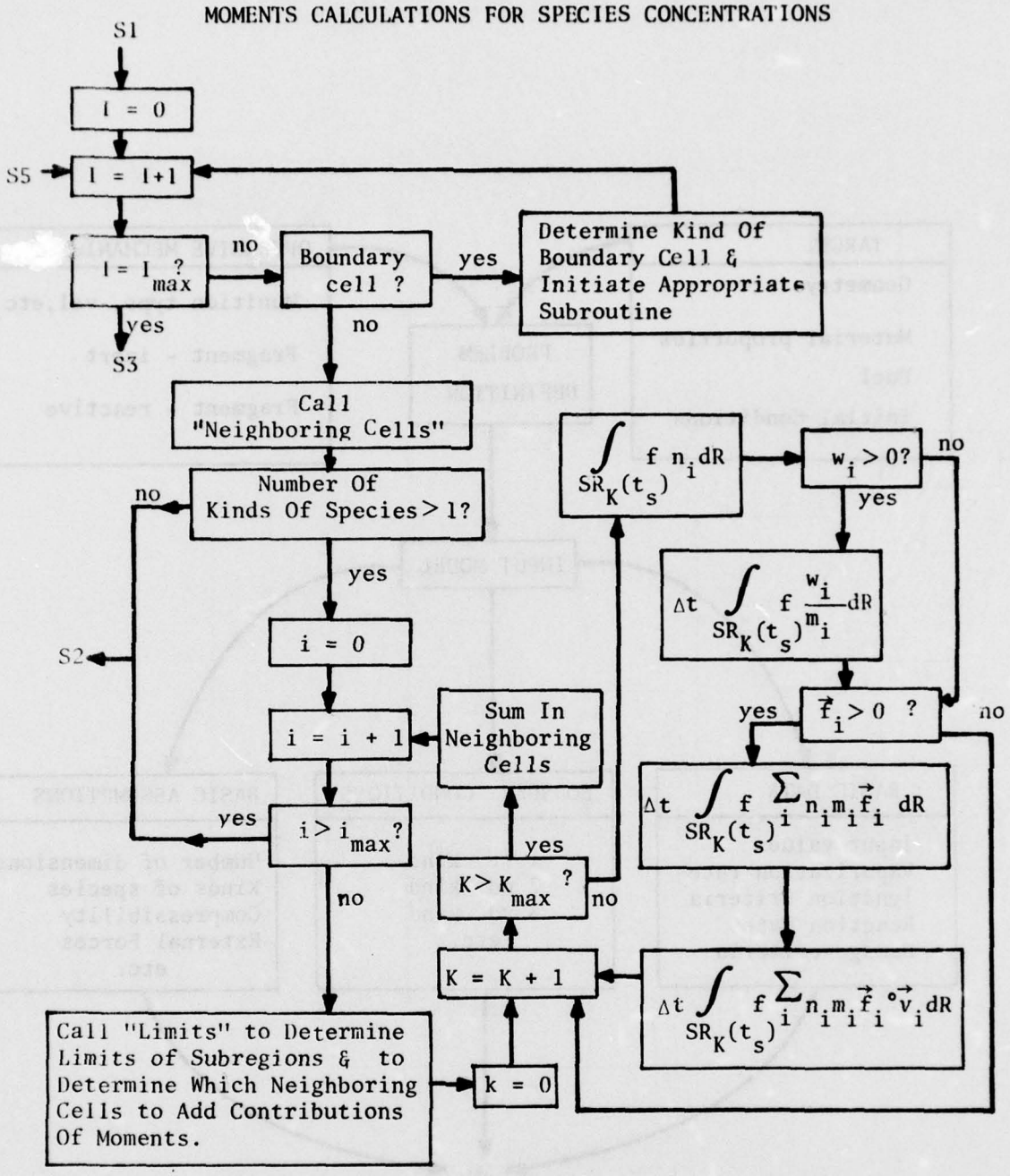


Figure IV-2 Flowchart For Code Construction (Continued).

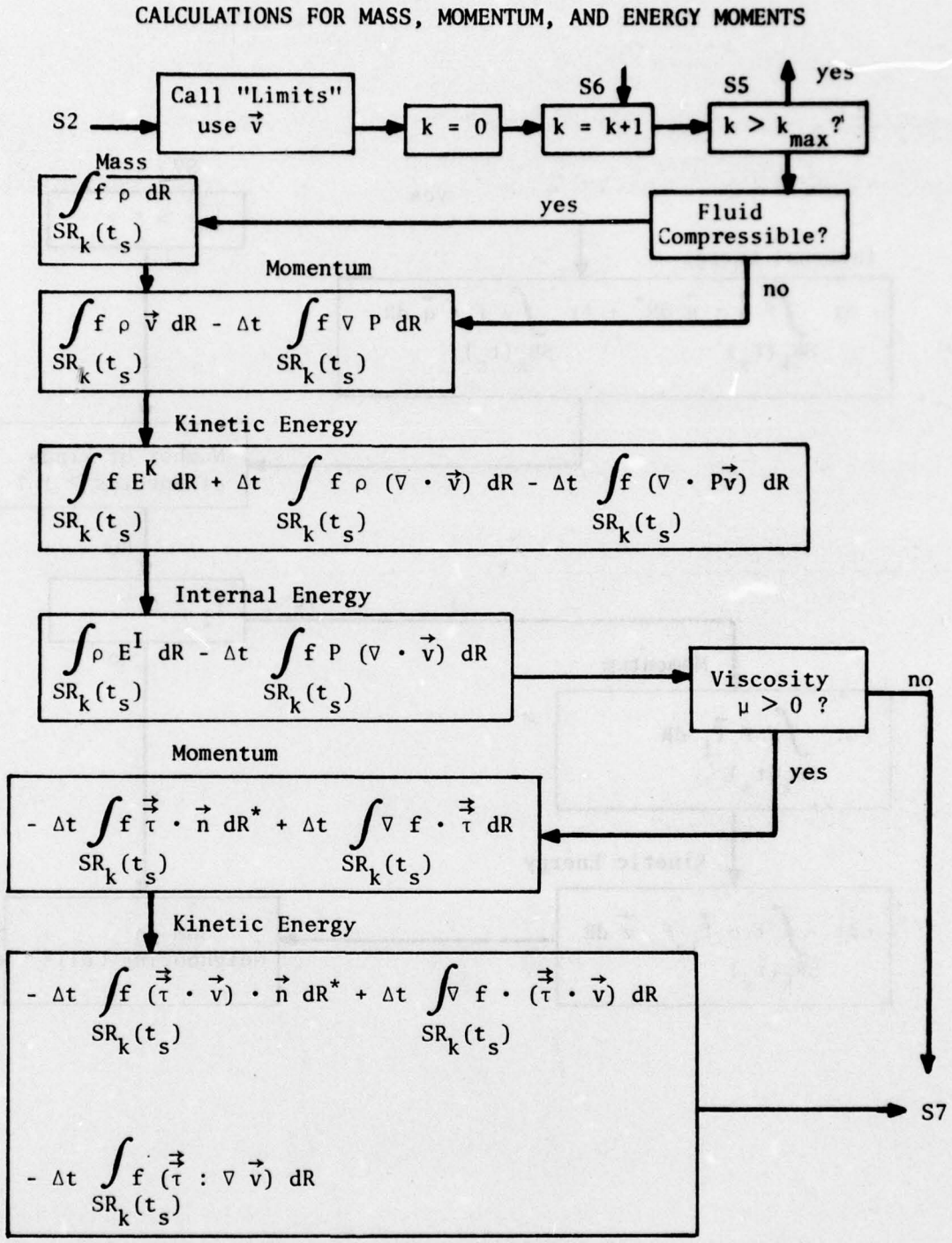


Figure IV-3 Flowchart For Code Construction (Continued)

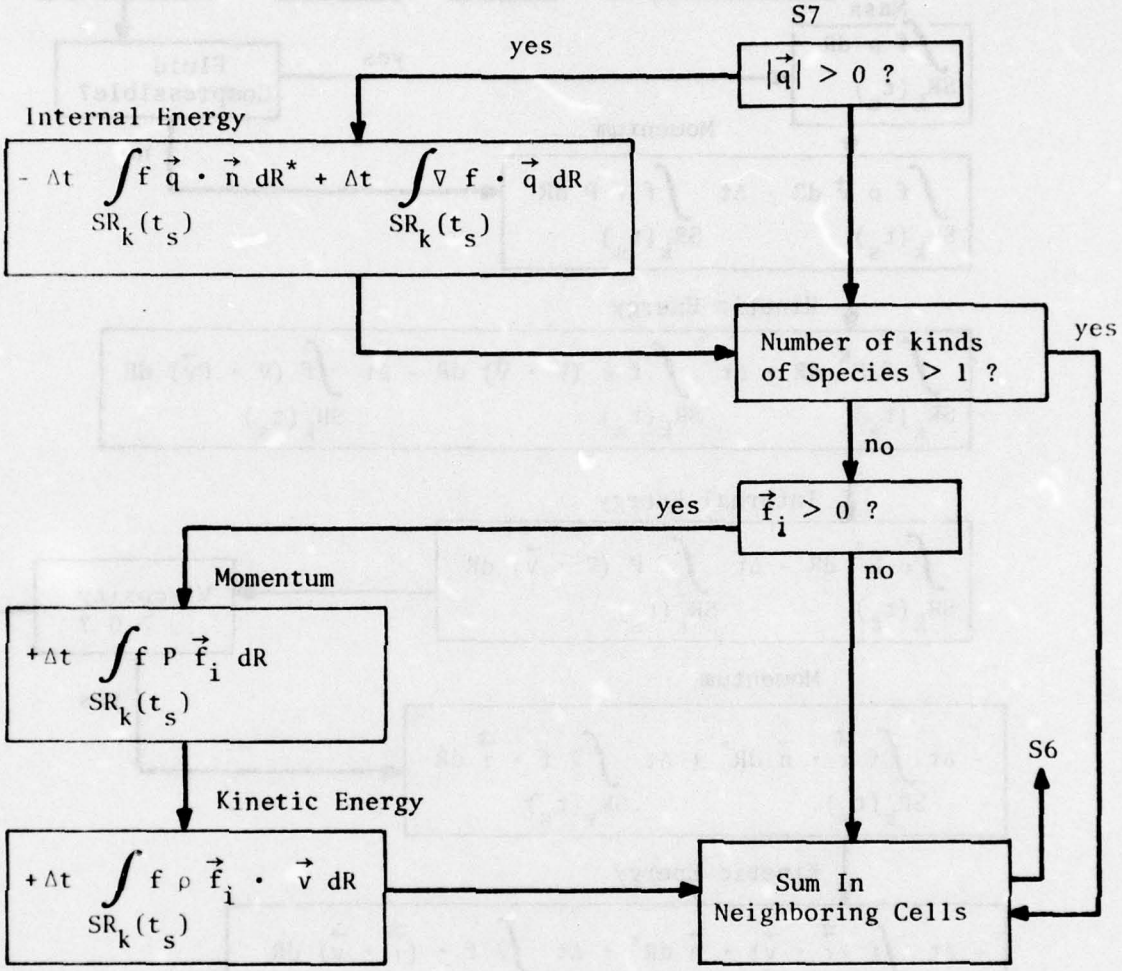


Figure IV-4 Flowchart For Code Construction (Continued).

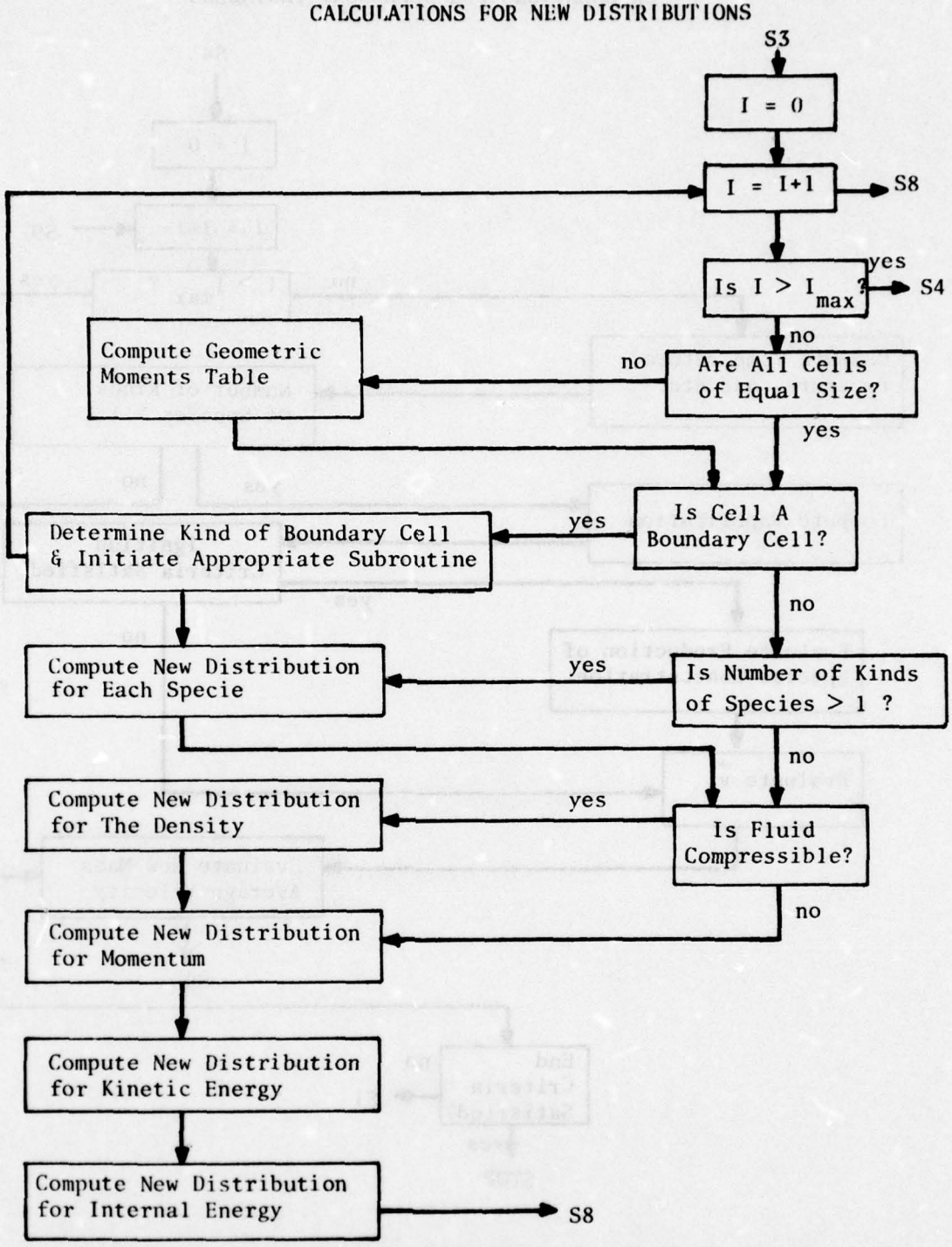


Figure IV-5 Flowchart For Code Construction (Continued).

CALCULATIONS FOR DEPENDENT VARIABLES

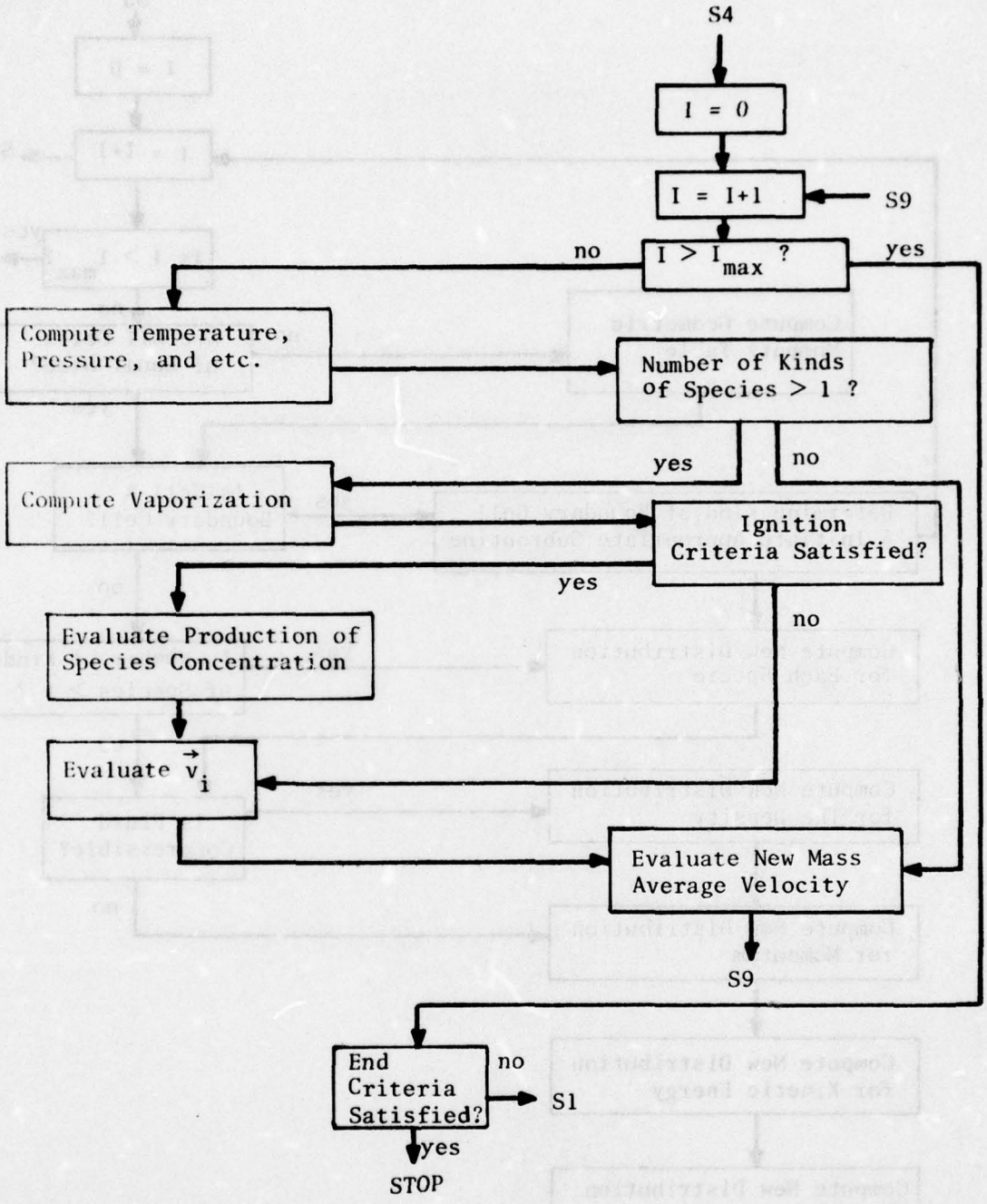


Figure IV-6 Flowchart For Code Construction (Continued).

In the case of two dimensional flow, there will be nine neighboring cells including the current I cell.

The next step is to determine if there are more than one kind of species. In the case of one kind of species, the code would proceed to S2 of the flowchart as shown in Figure IV-3. If not, then the code would initiate a reiteration design to compute the moments of the species concentration for each i kind of species. Each kind of species will have associated with it a velocity distribution $\vec{v}_i$. Consequently, a Lagrangian cell of that species would be calculated to move according to $\vec{v}_i$ and limits of subregions SR_K at t_s would be determined by a subroutine entitled "Limits" in the flowchart. In addition, subroutine "Limits" would identify the neighboring cells in which the moments of the subregions are to be summed. Then taking each subregion in turn, the moments for the species concentration would be calculated and summed. In this procedure some of the subroutines would be bypassed if $w_i = 0$ or if $\vec{f}_i = 0$. After all of the kinds of species have been considered, the code would move on to consider the remaining physical parameters, where the flowchart is marked with the symbol S2.

In considering the computation of moments for the remaining physical parameters, in Figure IV-3, it is noted that subroutine "Limits" would again be called and, based on the mass average velocity, the limits of subregions at t_s would be determined. Following the flowchart, it can be seen that if the fluid is assumed to be incompressible, the integral for computing the mass moments would be bypassed. Then the terms for calculating the moments for momentum and energy would be evaluated. However certain terms may be bypassed if the viscosity is zero, the heat flux is zero, the number of kinds of species is greater than one, or if exterior forces are absent. Once all of the subregions have been accounted for, the code would recycle until all of the cells have been processed. At the conclusion of these calculations, corresponding to each of the I cells, there will be sums of the various moments stored.

The new distributions of the physical quantities at $t_s + \Delta t$ would be determined by the operations presented in Figure IV-5. As before in the case of boundary cells, special subroutines would be called to impose the appropriate boundary conditions. If the size of the cells varies from one cell to another, then for each cycle of computation the Geometric Moments would have to be computed for the different size cells or a table of these values required. If the cell sizes vary in the computation, then appropriate adjustments in the table would be needed to reflect these changes. At the completion of these calculations, the new distributions of the physical parameters at $t_s + \Delta t$ would be available for the next cycle of computation.

In Figure IV-6, some of the operations which would be needed to complete the calculation are presented. Firstly, certain physical quantities may be required which depend on those already calculated. These could include fluid temperature and pressure. If more than one

kind of species is possible, then based on the ignition criteria, it would be determined if ignition had occurred. If so, then a new value of w_i (the mass rate of production term) based on the existing temperature and species concentrations would be evaluated for use in the next cycle. Afterwards a new species velocity, for each species, would be determined from which a new mass average velocity could be derived. At this point, the code would be prepared to print out data, initiate the next cycle or stop.

The flowchart does not indicate numerous operations and subroutines which the final version of the code will need. In some cases it will be desirable to change the cell sizes by doubling or halving some or all of them. A difficulty will be the programing of the code such that arbitrary coordinates systems can be handled (cartesian, cylindrical, spherical, etc). Also certain problems must be resolved, such as ensuring that distributions of physical quantities are continuous across cell boundaries and that non-negative quantities never end up with negative values. In order to place these and possibly other problem areas in perspective relative to the entire code, the flowchart needs to be expanded. However, the current version provides sufficient descriptive information to adequately portray the basic approach for organizing the code structure.

V. CONCLUSIONS

The objective of this report is to document the essential and basic elements of the proposed mathematical and physical scheme for simulating fluid flow. The simple problem solved in Section III provides verification to the extent that it demonstrates that the approach is feasible. The flowchart and its associated description in Section IV provides a general picture as to a possible procedure for implementing the proposed method in terms of a computer code. There is no attempt to anticipate or categorize all of the difficult areas or to explain how they might be overcome. That would tend to confuse and undermine the primary objective of the report.

The proposed method has two important characteristics. One is that it involves integral equations, which means that singular points will not be a problem and no instabilities will occur for that reason. The other is that the various physical parameters will be represented by variable distributions across the cells, which should provide increase accuracy in contrast to using constant distributions for the same cell size.

At this stage, it is impossible to make a reasonable comparison of this method with existing hydrodynamic codes which utilize other methods. This can be accomplished only when a code has been written and computational results compared. There is no way to estimate the computer time required to compute a typical problem. That also must be held in

abeyance until problems are run. To this end, progress in code construction will be accomplished as manpower and funds become available.

APPENDIX A

THE DETERMINATION OF DISTRIBUTIONS OF FUNCTIONS BY THE MOMENTS METHOD

A part of the mathematical basis of the theory is the so called Moments Method for the determination of an average distribution of a variable over a region if certain moments of the variable over sub-regions are known. The method may be derived directly from the concept of a weighted arithmetic mean. In general, if it is assumed that there are available $\alpha_1, \alpha_2, \ldots\ldots \alpha_J$ non-negative numbers (weights), not all zero, the weighted arithmetic mean $\bar{f}$ of $f_1, f_2, \ldots, f_J$ is defined by the following formula:

$$\bar{f} = \frac{\sum_J \alpha_J \, f_J}{\sum_J \alpha_J} \quad . \tag{A-1}$$

When the weights are all equal, Equation A-1 reduces to the expression for computing the ordinary arithmetic means.

This may be extended to the weighting of a function over an interval where the weighting function varies continuously. This extention yields the following equation:

$$\overline{f(x)} = \frac{\int \alpha(x) \, f(x) \, dx}{\int \alpha(x) \, dx} \tag{A-2}$$

where $\alpha(x)$ is a non-negative weighting function whose integral is not zero.

In Figure A-1, a function $\alpha(x)$, whose first derivative is discontinuous at certain values of x is plotted. Between each pair of first derivative discontinuity values, the function f(x) and the weight function $\alpha(x)$ are assumed to be known. Utilizing this information and Equation A-2, the following expression can be obtained:

$$\bar{f} = \frac{\int_{x_1}^{x_2} \alpha_1 \, f \, dx + \int_{x_2}^{x_3} \alpha_2 \, f \, dx + \ldots + \int_{x_5}^{x_6} \alpha_5 \, f \, dx}{\int_{x_1}^{x_2} \alpha_1 \, dx + \int_{x_2}^{x_3} \alpha_2 \, dx + \ldots + \int_{x_5}^{x_6} \alpha_5 \, dx} \quad . \tag{A-3}$$

Also indicated in Figure A-1, by the dashed line, is the average weight function for the entire range of x. The integral of the average weight function over the entire range of x is equivalent to the sum of the integrals of the individual weight functions over their corresponding intervals of x. That is

$$\int_{x_1}^{x_6} \alpha(x) \, dx = \int_{x_1}^{x_2} \alpha_1 \, dx + \int_{x_2}^{x_3} \alpha_2 \, dx + \ldots + \int_{x_5}^{x_6} \alpha_5 \, dx. \tag{A-4}$$

Also, we may write

$$\bar{f} = \frac{\int_{x_1}^{x_6} \alpha(x) \, f(x) \, dx}{\int_{x_1}^{x_6} \alpha(x) \, dx} \tag{A-5}$$

Combining Equations A-3, A-4, and A-5 yields the desired expression for evaluating the average weighting function $\alpha(x)$, written as follows:

$$\int_{x_1}^{x_2} \alpha_1 \, f \, dx + \int_{x_2}^{x_3} \alpha_2 \, f \, dx + \ldots + \int_{x_5}^{x_6} \alpha_5 \, f \, dx = \int_{x_1}^{x_6} \alpha \, f \, dx \tag{A-6}$$

where α_J and f are known. If f is set equal to $x^0 = 1$, then α is a constant as indicated in Figure A-1. However, f may be any power of x and for that reason α can be evaluated as a variable function. In two or three dimensions, f may be a function of the other spatial parameters as well.

For the purpose of demonstration, we may utilize Figure A-2, where a two dimensional spatial region is defined and which is partitioned into five subregions SR_J. Also, we may assume that corresponding to each subregion a known distribution of a physical parameter $\alpha(x,y)$ exist.

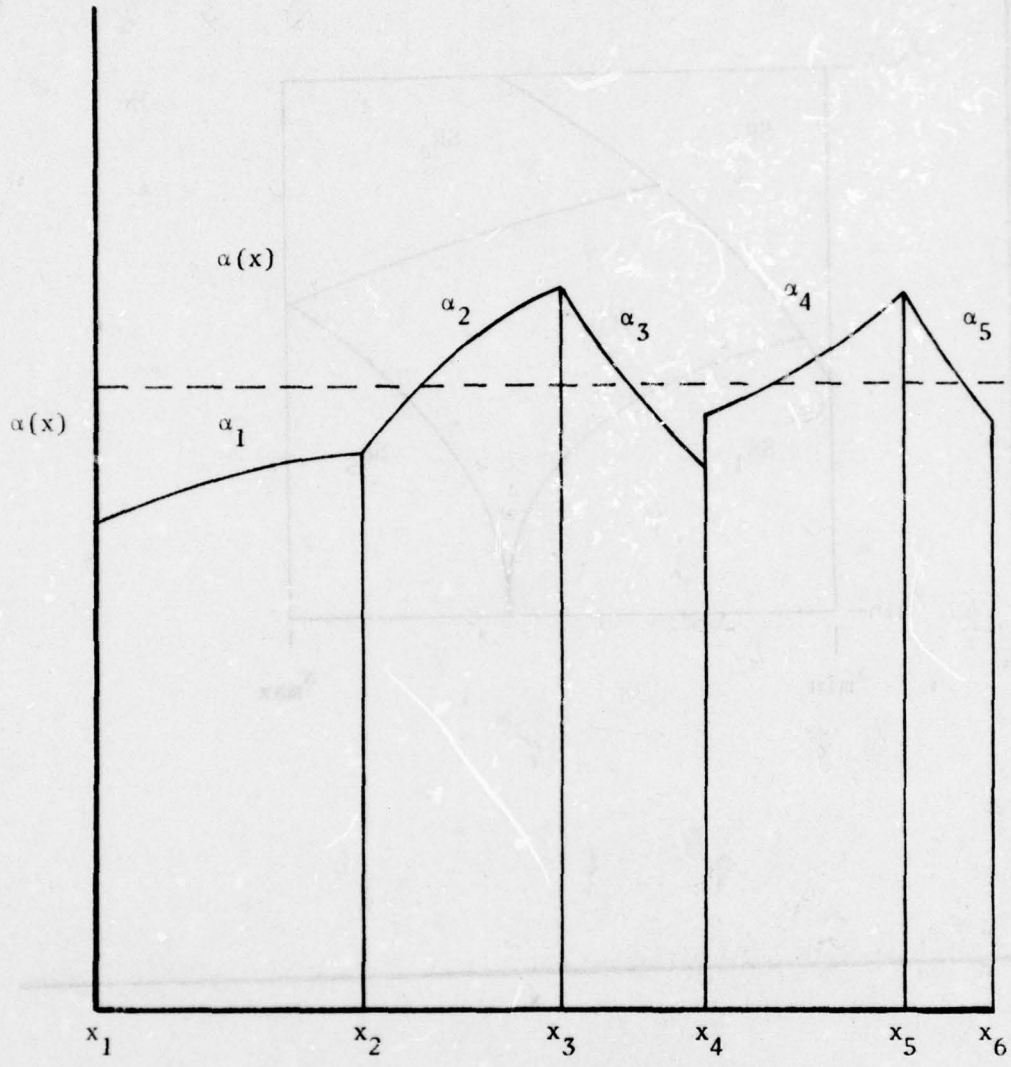


Figure A-1 Schematic Presentation Of An Average Function Based On Moments Over Subregions.

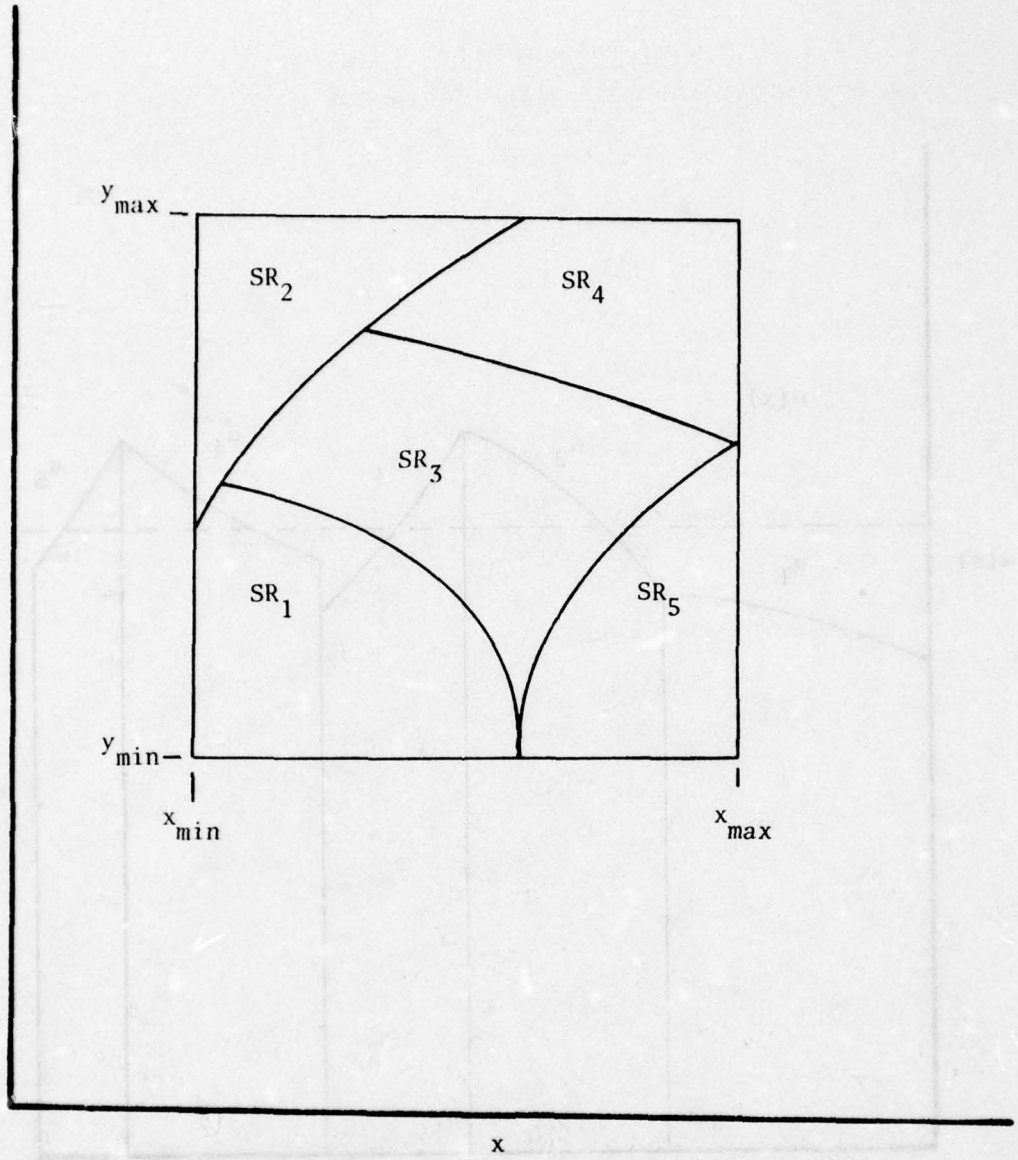


Figure A-2 Schematic Representation Of Subregions Of A Spatial Region Over Which Distributions Of A Physical Quantity Are Known.

Thus the weighting function is represented by $\alpha(x,y)_J$ and the function to be weighted is

$$f(x,y) = x^{k_1} y^{k_2} . \qquad \text{(A-7)}$$

Let's assume that the average weighting function $\alpha(x,y)$ is represented by the following equation:

$$\alpha(x,y) = b_1 x + b_2 y + b_3 \qquad \text{(A-8)}$$

where b_1, b_2, and b_3 are constants to be evaluated in the manner to be explained below.

By utilizing Equations A-6, A-7, and A-8 and setting the values of k_1 and k_2 to 1 and 0 respectively such that f = 1, x, or y, the following three equations are obtained:

$$\int_{SR_1} \alpha_1 \, dA + \int_{SR_2} \alpha_2 \, dA + \ldots . + \int_{SR_5} \alpha_5 \, dA = \int_{TC} \alpha \, dA$$

$$\int_{SR_1} \alpha_1 \, x \, dA + \int_{SR_2} \alpha_2 \, x \, dA + \ldots . + \int_{SR_5} \alpha_5 \, x \, dA = \int_{TC} \alpha \, x \, dA \qquad \text{(A-9)}$$

$$\int_{SR_1} \alpha_1 \, y \, dA + \int_{SR_2} \alpha_2 \, y \, dA + \ldots . + \int_{SR_5} \alpha_5 \, y \, dA = \int_{TC} \alpha \, y \, dA$$

where

$$\int_{TC} = \int_{y_{min}}^{y_{max}} \int_{x_{min}}^{x_{max}}$$

and $dA = dx \, dy$.

The integrals on the left of Equations A-9 can be evaluated once the limits of the subregions have been determined. By summing the values of those integrals and substituting from Equations A-8, the following form of the equations is obtained:

$$\sum_J \int_{SR_J} \alpha_J \, dA = b_1 \int_{TC} x \, dA + b_2 \int_{TC} y \, dA + b_3 \int_{TC} dA$$

$$\sum_J \int_{SR_J} x \, \alpha_J \, dA = b_1 \int_{TC} x^2 \, dA + b_2 \int_{TC} x \, y \, dA + b_3 \int_{TC} x \, dA \qquad \text{(A-10)}$$

$$\sum_J \int_{SR_J} y \, \alpha_J \, dA = b_1 \int_{TC} x \, y \, dA + b_2 \int_{TC} y^2 \, dA + b_3 \int_{TC} y \, dA \, .$$

The integrals on the right side of Equations A-10 depend entirely on the spatial parameters, so for convenience, these integrals are referred to as Geometric Moments and are integrated over the entire spatial region. Since there are three equations and three unknowns, the coefficients b_1, b_2, and b_3 of α can be evaluated by solving the equations simultaneously. If higher order expressions for α are desired, the additional coefficients required can be evaluated by increasing the value of the k's in Equation A-7 and thereby increasing the number of Equations in A-10 accordingly.

APPENDIX B

THE DERIVATION OF THE INTEGRAL EQUATIONS FOR CALCULATING MOMENTS IN FLUID FLOW

In deriving the integral equations for computing moments of physical quantities over a spatial domain, where the results include changes over a time step Δt, it is sufficient to begin with the basic equations of change, written as follows:

Species Concentration:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \vec{v}_i = \frac{w_i}{m_i} \tag{B-1a}$$

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0 \tag{B-1b}$$

Momentum:

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho \vec{v})\, \vec{v} = - \nabla P - (\nabla \cdot \vec{\vec{\tau}}) + \sum_i n_i m_i \vec{f}_i \tag{B-1c}$$

Total Energy:

$$\frac{\partial E^T}{\partial t} + \nabla \cdot \vec{v} E^T = - \nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v}) - (\nabla \cdot P\vec{v}) - (\nabla \cdot \vec{q}) + \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i \tag{B-1d}$$

Kinetic Energy:

$$\frac{\partial E^K}{\partial t} + \nabla \cdot E^K \vec{v} = - \nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v}) + (\vec{\vec{\tau}} : \nabla \vec{v}) + P(\nabla \cdot \vec{v}) - \nabla \cdot P\vec{v} + \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i \tag{B-1e}$$

Internal Energy:

$$\frac{\partial E^I}{\partial t} + \nabla \cdot E^I \vec{v} = - \nabla \cdot \vec{q} - \vec{\vec{\tau}} : \nabla \vec{v} - P\,(\nabla \cdot \vec{v})\,. \tag{B-1f}$$

The definitions of the physical quantities used in Equations B-1 are listed as follows:

n_i - the number desity of the i^{th} species.

w_i - the mass rate of production of the i^{th} species through chemical reactions.

$\vec{v}_i$ - the average velocity of the i^{th} species.

m_i - the mass of the i^{th} species.

ρ - the mass per unit volume (density).

$\vec{v}$ - the mass average velocity of the mixture.

P - the pressure.

$\vec{\vec{\tau}}$ - the stress tensor.

$\vec{f}_i$ - the external force per unit mass on the i^{th} species.

E^T - the total energy.

$\vec{q}$ - the energy flux.

E^K - the kinetic energy ($1/2\ \rho\ \vec{v}^2$).

E^I - the internal energy.

The conservation laws, in integral form, are to be applied to fluid volumes which move through a fixed coordinate system. In addition, weight functions are utilized and these are assumed to be products of powers of x, y, and z at $t = t_s + \Delta t$ and in addition satisfy the following differential equation.

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = 0 \ . \qquad \text{(B-2)}$$

In deriving the necessary form of the equations, the function f is initially multiplied through Equations B-1. Substitution and rearrangement of the terms yields the following form:

Species Concentration:

$$\frac{\partial f n_i}{\partial t} + f\ (\nabla \cdot (n_i\ \vec{v}_i) = n_i \frac{\partial f}{\partial t} + f \frac{w_i}{m_i} \qquad \text{(B-3a)}$$

Mass:

$$\frac{\partial f\rho}{\partial t} + f\,(\nabla \cdot \rho\,\vec{v}) = \rho\,\frac{\partial f}{\partial t} \tag{B-3b}$$

Momentum:

$$\frac{\partial f\rho v}{\partial t} + f\,(\nabla \cdot (\rho\vec{v})\,\vec{v}) = \rho\vec{v}\,\frac{\partial f}{\partial t} - f\,\nabla P - f\,(\nabla \cdot \vec{\vec{\tau}}) + f \sum_i n_i\, m_i\, \vec{f}_i \tag{B-3c}$$

Total Energy:

$$\frac{\partial f E^T}{\partial t} + f\,\nabla \cdot \vec{v}\,E^T = E^T\,\frac{\partial f}{\partial t} - f\,\nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v}) - f\,(\nabla \cdot \vec{q}) - f\,(\nabla \cdot P\vec{v}) + f \sum_i n_i\, m_i\, \vec{f}_i \cdot \vec{v}_i \tag{B-3d}$$

Kinetic Energy:

$$\frac{\partial f E^K}{\partial t} + f\,(\nabla \cdot E^K\,\vec{v}) = E^K\,\frac{\partial f}{\partial t} - f\,(\nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v})) + f\,(\vec{\vec{\tau}} : \nabla\,\vec{v}) + f\,(P\,(\nabla \cdot \vec{v})) - f\,(\nabla \cdot P\vec{v}) + f \sum_i n_i\, m_i\, \vec{f}_i\,\vec{v}_i \tag{B-3e}$$

Internal Energy:

$$\frac{\partial f E^I}{\partial t} + f\,(\nabla \cdot E^I\,\vec{v}) = E^I\,\frac{\partial f}{\partial t} - f\,(\nabla \cdot \vec{q}) - f\,(\vec{\vec{\tau}} : \nabla\,\vec{v}) - f\,P\,(\nabla \cdot \vec{v}) \tag{B-3f}$$

The following identities can be used for transforming the above equations to the desired form:

$$U\,(\nabla \cdot V\vec{v}) = U\,(\nabla\,V \cdot \vec{v}) + U\,(V\,\nabla \cdot \vec{v}) \tag{B-4a}$$

and $$\nabla \cdot UV\vec{v} = V(\nabla U \cdot \vec{v}) + U(\nabla \cdot \vec{v}) + UV(\nabla \cdot \vec{v})$$ (B-4b)

or $$U \nabla V \cdot \vec{v} = (\nabla \cdot UV\vec{v}) - (V \nabla U \cdot \vec{v}) - (UV \nabla \cdot \vec{v})$$

and $$\nabla \cdot UV\vec{v} = UV(\nabla \cdot \vec{v}) + (\vec{v} \cdot \nabla UV)$$ (B-4c)

where U and V are arbitrary functions.

Substitution of Equations B-4 into Equations B-3 and after rearrangement of terms, the following equations are obtained:

Species Concentration:

$$\frac{\partial fm_i}{\partial t} + \vec{v}_i \cdot \nabla fn_i + fn_i (\nabla \cdot \vec{v}_i) = n_i (\frac{\partial f}{\partial t} + \vec{v}_i \cdot \nabla f) + f \frac{w_i}{m_i}$$ (B-5a)

Mass:

$$\frac{\partial f\rho}{\partial t} + \vec{v} \cdot \nabla f\rho + f\rho (\nabla \cdot \vec{v}) = \rho(\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f)$$ (B-5b)

Momentum:

$$\frac{\partial f\rho\vec{v}}{\partial t} + \vec{v} \cdot \nabla f\rho\vec{v} + f\,\rho\vec{v}\,(\nabla \cdot \vec{v}) = \rho\,\vec{v}\,(\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f)$$
$$- f\,(\nabla \cdot \vec{\tau}) - f\,\nabla P + f \sum_i n_i\, m_i\, \vec{f}_i$$ (B-5c)

Total Energy:

$$\frac{\partial fE^T}{\partial t} + \vec{v} \cdot \nabla f\,E^T + f\,E^T\,(\nabla \cdot \vec{v}) = E^T\,(\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f) - f\,(\nabla \cdot (\vec{\tau} \cdot \vec{v}))$$
$$- f(\nabla \cdot \vec{q}) - f(\nabla \cdot P\,\vec{v}) + f \sum_i n_i\, m_i\, \vec{f}_i \cdot \vec{v}_i$$ (B-5d)

Kinetic Energy:

$$\frac{\partial f E^K}{\partial t} + \vec{v} \cdot \nabla f E^K \; (\nabla \cdot \vec{v}) = E^K \left(\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f\right)$$

$$- f \nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v}) + f \; (\vec{\vec{\tau}} : \nabla \vec{v}) + f \, P \; (\nabla \cdot \vec{v}) \qquad \text{(B-5e)}$$

$$- f \; (\nabla \cdot P\vec{v}) + f \sum_i n_i \, m_i \, \vec{f}_i \cdot \vec{v}_i$$

Internal Energy:

$$\frac{\partial f E^I}{\partial t} + \vec{v} \cdot \nabla f E^I \; (\nabla \cdot \vec{v}) = E^I \left(\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f\right) \qquad \text{(B-5f)}$$

$$- f \; (\nabla \cdot \vec{q}) - f \; (\vec{\vec{\tau}} : \nabla \vec{v}) - f \, P \; (\nabla \cdot \vec{v})$$

The substantial derivative (also referred to as the derivative following the motion) D/DT is defined as the change with respect to time plus the change with respect to position. That is:

$$\frac{D(UV)}{Dt} = \frac{\partial (UV)}{\partial t} + \vec{v} \cdot \nabla \, UV \qquad \text{(B-6)}$$

Substitution of the substantial derivative into Equations B-5 and then integrating the terms over a spatial domain R(t), which has a bounding surface $R^*(t)$, yields the following set of integral equations:

Species Concentration:

$$\int_{R(t)} \left[\frac{D \, f \, n_i}{Dt} + f \, n_i \; (\nabla \cdot \vec{v}_i)\right] dR = \int_{R(t)} n_i \left[\frac{\partial f}{\partial t} + (\vec{v}_i \cdot \nabla f)\right] dR \qquad \text{(B-7a)}$$

$$+ \int_{R(t)} f \, \frac{w_i}{m_i} \, dR$$

Mass:

$$\int_{R(t)} \left[\frac{Df\rho}{Dt} + f\rho\,(\nabla \cdot \vec{v}) \right] dR = \int_{R(t)} \rho \left[\frac{\partial f}{\partial t} + (\vec{v} \cdot \nabla f) \right] dR \qquad \text{(B-7b)}$$

Momentum:

$$\int_{R(t)} \left[\frac{Df\rho v}{Dt} + f\rho\,\vec{v}\,(\nabla \cdot \vec{v}) \right] dR = \int_{R(t)} \rho\,\vec{v} \left[\frac{\partial f}{\partial t} + (\vec{v} \cdot \nabla f) \right] dR$$

$$- \int_{R(t)} f\,(\nabla \cdot \vec{\tau})\,dR - \int_{R(t)} f\,\nabla P\,dR + \int_{R(t)} f \sum_i n_i m_i \vec{f}_i\,dR \qquad \text{(B-7c)}$$

Total Energy:

$$\int_{R(t)} \left[\frac{DfE^T}{Dt} + fE^T\,(\nabla \cdot \vec{v}) \right] dR = \int_{R(t)} E^T \left[\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f \right] dR$$

$$- \int_{R(t)} f\,\nabla \cdot (\vec{\tau} \cdot \vec{v})\,dR - \int_{R(t)} f\,(\nabla \cdot \vec{q})\,dR \qquad \text{(B-7d)}$$

$$- \int_{R(t)} f\,(\nabla \cdot P\,\vec{v})\,dR + \int_{R(t)} f \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i\,dR$$

Kinetic Energy:

$$\int_{R(t)} \left[\frac{DfE^K}{Dt} - fE^K\,(\nabla \cdot \vec{v}) \right] dR = \int_{R(t)} E^K \left[\frac{\partial f}{\partial t} + (\vec{v} \cdot \nabla f \right] dR$$

$$- \int_{R(t)} f\,[\nabla \cdot (\vec{\tau} \cdot \vec{v})]\,dR + \int_{R(t)} f\,(\vec{\tau} : \nabla\,\vec{v})\,dR \qquad \text{(B-7e)}$$

(continued)

$$+ \int_{R(t)} f\, P\, (\nabla \cdot \vec{v})\, dR - \int_{R(t)} f\, (\nabla \cdot P\, \vec{v})\, dR \qquad \text{(B-7e cont)}$$

$$+ \int_{R(t)} f \sum_i n_i\, m_i\, \vec{f}_i \cdot \vec{v}_i\, dR$$

Internal Energy:

$$\int_{R(t)} \left[\frac{Df E^I}{Dt} + f\, E^I\, (\nabla \cdot \vec{v}) \right] dR = \int_{R(t)} E^I \left[\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f \right] dR$$

$$- \int_{R(t)} f\, (\nabla \cdot \vec{q})\, dR - \int_{R(t)} f\, (\vec{\tau} : \nabla \vec{v})\, dR \qquad \text{(B-7f)}$$

$$- \int_{R(t)} f\, P\, (\nabla \cdot \vec{v})\, dR$$

In order to transform Equations B-7, such that appropriate integral equations can be obtained, it is necessary to recall the Convection Theorm[2], given as follows:

$$\frac{D}{Dt} \int_{R(t)} U\, dR = \int_{R(t)} \left[\frac{DU}{Dt} + U\, (\nabla \cdot \vec{v}) \right] dR \qquad \text{(B-8)}$$

or

$$\frac{D}{Dt} \int_{R(t)} U\, dR = \frac{\partial}{\partial t} \int_{R(t)} U\, dR + \int_{R(t)} U\, (\vec{v} \cdot \vec{n})\, dR^* \qquad \text{(B-9)}$$

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[2] *Meyer, Richard E., "Introduction to Mathematical Fluid Dynamics," Wile Interscience, New York, N. Y., 1971.*

where $\vec{n}$ is a unit vector normal to the surface dR^*. For our purpose, the second term of Equation B-9 is set to zero since no fluid is to be permitted to cross the boundary of the cell. The application of this condition plus the imposition of the restriction as defined by Equation B-2 to Equations B-7 yields the following set of equations:

Species Concentration:

$$\frac{d}{dt} \int_{R(t)} f\, n_i \, dR = \int_{R(t)} f \frac{w_i}{m_i} \, dR \tag{B-10a}$$

Mass:

$$\frac{d}{dt} \int_{R(t)} f\, \rho \, dR \tag{B-10b}$$

Momentum:

$$\frac{d}{dt} \int_{R(t)} f\, \rho \vec{v} \, dR = - \int_{R(t)} f\, (\nabla \cdot \vec{\vec{\tau}}) \, dR - \int_{R(t)} f\, \nabla P \, dR + \int_{R(t)} f_i \sum_i n_i\, m_i\, \vec{f}_i \, dR \tag{B-10c}$$

Total Energy:

$$\frac{d}{dt} \int_{R(t)} f\, E^T \, dR = - \int_{R(t)} f\, \nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v}) \, dR - \int_{R(t)} f\, (\nabla \cdot \vec{q}) \, dR - \int_{R(t)} f\, (\nabla \cdot P\vec{v}) \, dR + \int_{R(t)} f \sum_i n_i\, m_i\, \vec{f}_i \cdot \vec{v}_i \, dR \tag{B-10d}$$

Kinetic Energy:

$$\frac{d}{dt}\int_{R(t)} f\,E^K\,dR = -\int_{R(t)} f\,\nabla\cdot(\vec{\vec{\tau}}\cdot\vec{v})\,dR + \int_{R(t)} f\,(\vec{\vec{\tau}}:\nabla\vec{v})\,dR$$

$$+\int_{R(t)} f\,P\,(\nabla\cdot\vec{v})\,dR - \int_{R(t)} f\,(\nabla\cdot P\vec{v})\,dR \qquad \text{(B-10e)}$$

$$+\int_{R(t)} f\,\sum_i n_i\,m_i\,\vec{f}_i\cdot\vec{v}_i\,dR$$

Internal Energy:

$$\frac{d}{dt}\int_{R(t)} f\,E^I\,dR = -\int_{R(t)} f\,(\nabla\cdot\vec{q})\,dR - \int_{R(t)} f\,(\vec{\vec{\tau}}:\nabla\vec{v})\,dR$$

$$-\int_{R(t)} f\,P\,(\nabla\cdot\vec{v})\,dR \qquad \text{(B-10f)}$$

Approximate solutions can be obtained by replacing Equations B-10 with the following equations:

Species Concentration:

$$\int_{R(t_s+\Delta t)} f\,n_i\,dR = \int_{R(t_s)} f\,n_i\,dR + \Delta t\int_{R(t_s)} f\,\frac{w_i}{m_i}\,dR \qquad \text{(B-11a)}$$

Mass:

$$\int_{R(t_s+\Delta t)} f\,\rho\,dR = \int_{R(t_s)} f\,\rho\,dR \qquad \text{(B-11b)}$$

Momentum:

$$\int_{R(t_s + \Delta t)} f \rho \vec{v}\, dR = \int_{R(t_s)} f \rho \vec{v}\, dR - \Delta t \int_{R(t_s)} f (\nabla \cdot \vec{\vec{\tau}})\, dR$$

$$- \Delta t \int_{R(t_s)} f \nabla P\, dR + \Delta t \int_{R(t_s)} f \sum_i n_i m_i \vec{f}_i\, dR \qquad \text{(B-11c)}$$

Total Energy:

$$\int_{R(t_s + \Delta t)} f E^T\, dR = \int_{R(t_s)} f E^T\, dR - \Delta t \int_{R(t_s)} f [\nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v})]\, dR$$

$$- \Delta t \int_{R(t_s)} f (\nabla \cdot \vec{q})\, dR - \Delta t \int_{R(t_s)} f (\nabla \cdot P\vec{v})\, dR \qquad \text{(B-11d)}$$

$$+ \Delta t \int_{R(t_s)} f \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i\, dR$$

Kinetic Energy:

$$\int_{R(t_s + \Delta t)} f E^K\, dR = \int_{R(t_s)} f E^K\, dR - \Delta t \int_{R(t_s)} \nabla \cdot (\vec{\vec{\tau}} \cdot \vec{v})\, dR$$

$$+ \Delta t \int_{R(t_s)} f (\vec{\vec{\tau}} : \nabla \vec{v})\, dR + \Delta t \int_{R(t_s)} f P (\nabla \cdot \vec{v})\, dR \qquad \text{(B-11e)}$$

$$- \Delta t \int_{R(t_s)} f (\nabla \cdot P\vec{v})\, dR + \Delta t \int_{R(t_s)} f \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i\, dR$$

Internal Energy:

$$\int_{R(t_s + \Delta t)} f E^I \, dR = \int_{R(t_s)} f E^I \, dR - \Delta t \int_{R(t_s)} f (\nabla \cdot \vec{q}) \, dR$$

$$- \Delta t \int_{R(t_s)} f (\vec{\vec{\tau}} : \nabla \vec{v}) \, dR - \Delta t \int_{R(t_s)} f P (\nabla \cdot \vec{v}) \, dR \qquad \text{(B-11f)}$$

The following expressions are required to obtain the desired form of the equations:

$$\int_{R(t_s)} \nabla \cdot U \vec{v} \, dR = \int_{R(t_s)} U (\nabla \cdot \vec{v}) \, dR + \int_{R(t_s)} \nabla U \cdot \vec{v} \, dR \qquad \text{(B-12a)}$$

and the Divergence Theorem:

$$\int_{R(t_s)} U (\nabla \cdot \vec{v}) \, dR = \int_{R^*(t_s)} U \vec{v} \cdot \vec{n} \, dR^* \qquad \text{(B-12b)}$$

Application of Equation B-12 to Equations B-11 yields the final form of the integral equations written as follows:

Species Concentration:

$$\int_{R(t_s + \Delta t)} f n_i \, dR = \int_{R(t_s)} f n_i \, dR + \Delta t \int_{R(t_s)} f \frac{w_i}{m_i} \, dR \qquad \text{(B-13a)}$$

Mass:

$$\int_{R(t_s + \Delta t)} f \rho \, dR = \int_{R(t_s)} f \rho \, dR \qquad \text{(B-13b)}$$

Momentum:

$$\int_{R(t_s + \Delta t)} f \rho \vec{v} \, dR = \int_{R(t_s)} f \rho \vec{v} \, dR - \Delta t \int_{R^*(t_s)} f \vec{\vec{\tau}} \cdot dR^*$$

$$+ \Delta t \int_{R(t_s)} \nabla f \cdot \vec{\vec{\tau}} \, dR - \Delta t \int_{R(t_s)} f \nabla P \, dR + \Delta t \int_{R(t_s)} f \sum_i n_i m_i \vec{f}_i \, dR \qquad \text{(B-13c)}$$

Total Energy:

$$\int_{R(t_s + \Delta t)} f E^T \, dR = \int_{R(t_s)} f E^T \, dR - \Delta t \int_{R^*(t_s)} f (\vec{\vec{\tau}} \cdot \vec{v}) \cdot \vec{n} \, dR^*$$

$$+ \Delta t \int_{R(t_s)} \nabla f \cdot (\vec{\vec{\tau}} \cdot \vec{v}) \, dR - \Delta t \int_{R^*(t_s)} f \vec{q} \cdot \vec{n} \, dR^* + \Delta t \int_{R(t_s)} \nabla f \cdot \vec{q} \, dR \qquad \text{(B-13d)}$$

$$- \Delta t \int_{R(t_s)} f (\nabla \cdot P \vec{v}) \, dR + \Delta t \int_{R(t_s)} f \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i \, dR$$

Kinetic Energy:

$$\int_{R(t_s + \Delta t)} f E^K \, dR = \int_{R(t_s)} f E^K \, dR - \Delta t \int_{R^*(t_s)} f (\vec{\vec{\tau}} \cdot \vec{v}) \, dR^*$$

$$+ \Delta t \int_{R(t_s)} \nabla f \cdot (\vec{\vec{\tau}} \cdot \vec{v}) \, dR + \Delta t \int_{R(t_s)} f (\vec{\vec{\tau}} : \nabla \vec{v}) \, dR$$

$$+ \Delta t \int_{R(t_s)} f P (\nabla \cdot \vec{v}) \, dR - \Delta t \int_{R(t_s)} f (\nabla \cdot \vec{v}) \, dR \qquad \text{(B-13e)}$$

$$+ \Delta t \int_{R(t_s)} f \sum_i n_i m_i \vec{f}_i \cdot \vec{v}_i \, dR$$

Internal Energy:

$$\int_{R(t_s + \Delta t)} f E^I \, dR = \int_{R(t_s)} f E^I \, dR - \Delta t \int_{R^*(t_s)} f \vec{q} \cdot \vec{n} \, dR^*$$

$$+ \Delta t \int_{R(t_s)} \nabla f \cdot \vec{q} \, dR - \Delta t \int_{R(t_s)} f (\vec{\vec{\tau}} : \nabla \vec{v}) \, dR \qquad \text{(B-13f)}$$

$$- \Delta t \int_{R(t_s)} f P (\nabla \cdot \vec{v}) \, dR \, .$$

These integral equations are sufficient to utilize for the computation of approximate values of moments of physical quantities related to fluid flow over a spatial domain in a time increment Δt.

APPENCIX C

DEVELOPMENT OF EXPRESSIONS FOR CALCULATING DENSITY, MOMENTUM AND KINETIC ENERGY DISTRIBUTION AT $t_s + \Delta t$ BASED ON THE MOMENTS

The form of the expression for calculating a distribution of a physical parameter over a spatial region is arbitrary provided the values of the required moments are available. Since the limits of the sub-regions are determined by the velocity distributions and it is desirable to simplify the integrations, the velocity distribution are assumed to be linear in form, as follows:

$$\vec{v}_x = \vec{i}\,(A(1,1)\ y + A(2,1)\ z + A(3,1))$$

$$\vec{v}_y = \vec{j}\,(A(1,2)\ z + A(2,2)\ x + A(3,2)) \qquad \text{(C-1)}$$

$$\vec{v}_z = \vec{k}\,(A(1,3)\ x + A(2,3)\ y + A(3,3))$$

where

$\vec{v}_x, \vec{v}_y, \vec{v}_z$ = the velocity components

$\vec{i}, \vec{j}, \vec{k}$ = unit orthogonal vectors

$A(i,j)$ = coefficients

x, y, z = spatial parameters in fixed coordinates.

The coefficients of Expressions C-1 cannot be evaluated directly, but must be evaluated from a knowledge of the density distribution and the momentum or the kinetic energy distribution. Consequently, the density is required to be a constant across the cell and the momentum distribution is a linear function similiar to Expressions C-1. The form of the kinetic energy distribution reflects the velocity squared term. To assist in writing down the equations the symbol G, which represents the Geometric Moments as presented in Table C-1, are utilized.

Table C-1. The Integrals for Calculating Geometric Moments*

$G(1,1) = \int y^0 z^0 \, dR_1$	$G(1,2) = \int z^0 x^0 \, dR_2$	$G(1,3) = \int x^0 y^0 \, dR_3$
$G(2,1) = \int y^1 z^0 \, dR_1$	$G(2,2) = \int z^1 x^0 \, dR_2$	$G(2,3) = \int x^1 y^0 \, dR_3$
$G(3,1) = \int y^2 z^0 \, dR_1$	$G(3,2) = \int z^2 x^0 \, dR_2$	$G(3,3) = \int x^2 y^0 \, dR_3$
$G(4,1) = \int y^3 z^0 \, dR_1$	$G(4,2) = \int z^3 x^0 \, dR_2$	$G(4,3) = \int x^3 y^0 \, dR_3$
$G(5,1) = \int y^4 z^0 \, dR_1$	$G(5,2) = \int z^4 x^0 \, dR_2$	$G(5,3) = \int x^4 y^0 \, dR_3$
$G(6,1) = \int y^0 z^1 \, dR_1$	$G(6,2) = \int z^0 x^1 \, dR_2$	$G(6,3) = \int x^0 y^1 \, dR_3$
$G(7,1) = \int y^1 z^1 \, dR_1$	$G(7,2) = \int z^1 x^1 \, dR_2$	$G(7,3) = \int x^1 y^1 \, dR_3$
$G(8,1) = \int y^2 z^1 \, dR_1$	$G(8,2) = \int z^2 x^1 \, dR_2$	$G(8,3) = \int x^2 y^1 \, dR_3$
$G(9,1) = \int y^3 z^1 \, dR_1$	$G(9,2) = \int z^3 x^1 \, dR_2$	$G(9,3) = \int x^3 y^1 \, dR_3$
$G(10,1) = \int y^4 z^1 \, dR_1$	$G(10,2) = \int z^4 x^1 \, dR_2$	$G(10,3) = \int x^4 y^1 \, dR_3$
$G(11,1) = \int y^0 z^2 \, dR_1$	$G(11,2) = \int z^0 x^2 \, dR_2$	$G(11,3) = \int x^0 y^2 \, dR_3$
$G(12,1) = \int y^1 z^2 \, dR_1$	$G(12,2) = \int z^1 x^2 \, dR_2$	$G(12,3) = \int x^1 y^2 \, dR_3$
$G(13,1) = \int y^2 z^2 \, dR_1$	$G(13,2) = \int z^2 x^2 \, dR_2$	$G(13,3) = \int x^2 y^2 \, dR_3$
$G(14,1) = \int y^3 z^2 \, dR_1$	$G(14,2) = \int z^3 x^2 \, dR_2$	$G(14,3) = \int x^3 y^2 \, dR_3$
$G(15,1) = \int y^4 z^2 \, dR_1$	$G(15,2) = \int z^4 x^2 \, dR_2$	$G(15,3) = \int x^4 y^2 \, dR_3$
$G(16,1) = \int y^0 z^3 \, dR_1$	$G(16,2) = \int z^0 x^3 \, dR_2$	$G(16,3) = \int x^0 y^3 \, dR_3$
$G(17,1) = \int y^1 z^3 \, dR_1$	$G(17,2) = \int z^1 x^3 \, dR_2$	$G(17,3) = \int x^1 y^3 \, dR_3$
$G(18,1) = \int y^2 z^3 \, dR_1$	$G(18,2) = \int z^2 x^3 \, dR_2$	$G(18,3) = \int x^2 y^3 \, dR_3$
$G(19,1) = \int y^3 z^3 \, dR_1$	$G(19,2) = \int z^3 x^3 \, dR_2$	$G(19,3) = \int x^3 y^3 \, dR_3$
$G(20,1) = \int y^4 z^3 \, dR_1$	$G(20,2) = \int z^4 x^3 \, dR_2$	$G(20,3) = \int x^4 y^3 \, dR_3$
$G(21,1) = \int y^0 z^4 \, dR_1$	$G(21,2) = \int z^0 x^4 \, dR_2$	$G(21,3) = \int x^0 y^4 \, dR_3$

*$dR_1 = dx\ dy\ dz$; $dR_2 = dy\ dz\ dx$; $dR_3 = dz\ dx\ dy$

The Mass

The mass distribution, assumed to be a constant across the cell, is represented by the following equation:

$$\rho = A' \tag{C-2}$$

where

ρ = the density

A' = constant distribution across cell.

After multiplying through by the function f and integrating, we have the following integral equation:

$$\sum_J \int_{SR_J} f\, \rho_J\, dR_1 = A' \int_{TC} f\, dR_1 \tag{C-3}$$

where

SR_J = limits over subregion contribution by the J Lagrangian cell.

TC = limits over total cell.

dR_1 = dx dy dz.

f = weighted function.

For f = 1, Equation C-3 becomes:

$$\sum_J \int_{SR_J} \rho_J\, dR_1 = A'\, G(1,1) \tag{C-4}$$

where G(1,1) is the Geometric Moment. The coefficient A' can be evaluated with Equation C-4 and thus the new constant density for the cell is determined.

The Momentum

The momentum distributions have components in the $\vec{i}$, $\vec{j}$, and $\vec{k}$ directions corresponding to the velocity distribution expressions of C-1. Therefore, we may write them down as follows:

$$\begin{aligned} \rho\, \vec{v}_x &= \vec{i}\, (B(1,1)\, y + B(2,1)\, z + B(3,1)) \\ \rho\, \vec{v}_y &= \vec{j}\, (B(1,2)\, z + B(2\ 2)\, x + B(3,2)) \\ \rho\, \vec{v}_z &= \vec{k}\, (B(1,3)\, x + B(2,3)\, y + B(3,3)). \end{aligned} \tag{C-5}$$

Multiplying through by f yields the following expressions:

$$f \rho \vec{v}_x = \vec{i} \, (B(1,1) \, f \, y + B(2,1) \, f \, z + B(3,1) \, f)$$
$$f \rho \vec{v}_y = \vec{j} \, (B(1,2) \, f \, z + B(2,2) \, f \, x + B(3,2) \, f) \qquad \text{(C-6)}$$
$$f \rho \vec{v}_z = \vec{k} \, (B(1,3) \, f \, x + B(2,3) \, f \, y + B(3,3) \, f)$$

where

$B(i,j)$ - the coefficients

$\vec{v}_x, \vec{v}_y, \vec{v}_z$ = velocity components

$\vec{i}, \vec{j}, \vec{k}$ = unit orthogonal vectors.

These equations dictate that f be assigned (1,y,z) for the $\vec{i}$ Component, (1,z,x) for the $\vec{j}$ Component, and (1,x,y) for the $\vec{k}$ Component. In addition, the order of integration is dx dy dz, dy dz dx, and dz dx dy for components $\vec{i}$, $\vec{j}$, and $\vec{k}$ respectively. Consequently, the expressions for obtaining the values of the coefficients of the three components of momentum are as follows:

$\vec{i}$ Component:

$$M(1,1) = B(1,1) \, G(2,1) + B(2,1) \, G(6,1) + B(3,1) \, G(1,1)$$
$$M(2,1) = B(1,1) \, G(3,1) + B(2,1) \, G(7,1) + B(3,1) \, G(2,1) \qquad \text{(C-7a)}$$
$$M(3,1) = B(1,1) \, G(7,1) + B(2,1) \, G(11,1) + B(3,1) \, G(6.1)$$

where

$$M(1,1 = \sum_J \int_{SR_J} (\rho \vec{v}_x)_J \, dR_1$$
$$M(2,1) = \sum_J \int_{SR_J} y \, (\rho \vec{v}_x)_J \, dR_1 \qquad \text{(C-7b)}$$
$$M(3,1) = \sum_J \int_{SR_J} z \, (\rho \vec{v}_x)_J \, dR_1$$

and the G's are substituted from Table C-1. Naturally, the coefficients B(1,1), B(2,1), and B(3,1) are to be evaluated by solving Equations

C-6a simultaneously. The symbol dR_1 is equal to dx dy dz as before.

$\vec{j}$ Component:

$$M(1,2) = B(1,2)\ G(2,2) + B(2,2)\ G(6,2) + B(3,2)\ G(1,2)$$

$$M(2,2) = B(1,2)\ G(3,2) + B(2,2)\ G(7,2) + B(3,2)\ G(2,2) \qquad \text{(C-8a)}$$

$$M(3,2) = B(1,2)\ G(7,2) + B(2,2)\ G(11,2) + B(3,2)\ G(6,2)$$

where

$$M(1,2) = \sum_J \int_{SR_J} (\rho\ \vec{v}_y)_J\ dR_2$$

$$M(2,2) = \sum_J \int_{SR_J} z\ (\rho\ \vec{v}_y)_J\ dR_2 \qquad \text{(C-8b)}$$

$$M(3,2) = \sum_J \int_{SR_J} x\ (\rho\ \vec{v}_y)_J\ dR_2$$

and the symbol dR_2 is equal to dy dz dx.

$\vec{k}$ Component:

$$M(1,3) = B(1,3)\ G(2,3) + B(2,3)\ G(6,3) + B(3,3)\ G(1,3)$$

$$M(2,3) = B(1,3)\ G(3,3) + B(2,3)\ G(7,3) + B(3,3)\ G(2,3) \qquad \text{(C-9a)}$$

$$M(3,3) = B(1,3)\ G(7,3) + B(2,3)\ G(11,3) + B(3,3)\ G(3,3)$$

where

$$M(1,3) = \sum_J \int_{SR_J} (\rho\ \vec{v}_z)_J\ dR_3$$

$$M(2,3) = \sum_J \int_{SR_J} x\ (\rho\ \vec{v}_z)_J\ dR_3 \qquad \text{(C-9b)}$$

$$M(3,3) = \sum_J \int_{SR_J} y\ (\rho\ \vec{v}_z)_J\ dR_3$$

where the symbol dR_3 is equal to dz dx dy.

The Kinetic Energy

The kinetic energy is not a vector quantity. However, since it is directly related to the velocity which is a vector quantity, we will refer to components of kinetic energy corresponding to the $\vec{i}$, $\vec{j}$, and $\vec{k}$ components of velocity. The fact that kinetic energy is equal to $1/2\ \rho\ \vec{v}^2$ is reflected in the six term expressions which follow:

$\vec{i}$ Component:

$$\tfrac{1}{2}\rho\,\vec{v}_x^{\,2} = C(1,1)y^2 + C(2,1)z^2 + C(3,1) + C(4,1)yz + C(5,1) + C(6,1)z$$

$\vec{j}$ Component:

$$\tfrac{1}{2}\rho\,\vec{v}_y^{\,2} = C(1,2)z^2 + C(2,2)x^2 + C(3,2) + C(4,2)zx + C(5,2)z + C(6,2)x \qquad \text{(C-10)}$$

$\vec{k}$ Component:

$$\tfrac{1}{2}\rho\,\vec{v}_z^{\,2} = C(1,3)x^2 + C(2,3)y^2 + C(3,3) + C(4,3)xy + C(5,3)x + C(6,3)y$$

where the C's are the coefficients to be evaluated.

Multiplying through Equations C-10 by the function f yields the following expressions:

$\vec{i}$ Component:

$$f(\tfrac{1}{2}\rho\,\vec{v}_x^{\,2}) = C(1,1)\ f\ y^3 + C(2,1)\ f\ z^2 + C(3,1)\ f + C(4,1)\ f\ yz + C(5,1)\ f\ y + C(6,1)\ f\ z$$

$\vec{j}$ Component:

$$f(\tfrac{1}{2}\rho\,\vec{v}_y^{\,2}) = C(1,2)\ f\ z^2 + C(2,2)\ f\ x^2 + C(3,2)\ f + C(4,2)\ f\ zx + C(5,2)\ f\ z + C(6,2)\ f\ x \qquad \text{(C-11)}$$

$\vec{k}$ Component:

$$f(\tfrac{1}{2}\rho\,\vec{v}_z^{\,2}) = C(1,3)\ f\ x^2 + C(2,3)\ f\ y^2 + C(3,3)\ f + C(4,3)\ f\ xy + C(5,3)\ f\ x + C(6,3)\ f\ y.$$

The appropriate substitutions for f in Equations C-11 are (1, y, z, y z, y^2, z^2), (1, z, x, zx, z^2, x^2), and (1, x, y, xy, x^2, y^2) for the $\vec{i}$, $\vec{j}$, and $\vec{k}$ components respectively. In addition, the order of integration is dx dy dz, dy dz dx, and dz dx dy for components $\vec{i}$, $\vec{j}$, and $\vec{k}$ respectively. Consequently, the expressions for obtaining the values of the coefficients of the components of kinetic energy are as follows:

$\vec{i}$ Component:

$$N(1,1) = C(1,1)\,G(3,1) + C(2,1)\,G(11,1) + C(3,1)\,G(1,1) + C(4,1)\,G(7,1) + C(5,1)\,G(2,1) + C(6,1)\,G(6,1)$$

$$N(2,1) = C(1,1)\,G(4,1) + C(2,1)\,G(12,1) + C(3,1)\,G(2,1) + C(4,1)\,G(8,1) + C(5.1)\,G(3,1) + C(6,1)\,G(7.1)$$

$$N(3,1) = C(1,1)\,G(8.1) + C(2,1)\,G(16,1) + C(3,1)\,G(6.1) + C(4,1)\,G(12,1) + C(5.1)\,G(7.1) + C(6,1)\,G(11,1)$$

$$N(4,1) = C(1,1)\,G(14,1) + C(2.1)\,G(17,1) + C(3.1)\,G(7.1) + C(4,1)\,G(13,1) + C(5.1)\,G(8,1) + C(6.1)\,G(12,1)$$

$$N(5,1) = C(1,1)\,G(5,1) + C(2,1)\,G(13,1) + C(3,1)\,G(3,1) + C(4,1)\,G(9,1) + C(5,1)\,G(4,1) + C(6,1)\,G(8,1)$$

$$N(6,1) = C(1,1)\,G(13,1) + C(2,1)\,G(21,1) + C(3,1)\,G(11,1) + C(4,1)\,G(17,1) + C(5,1)\,G(12,1) + C(6.1)\,G(16,1)$$

(C-12a)

where the G's are substituted from Table C-1, and

$$N(1,1) = \sum_J \iiint_{SR_J} (\tfrac{1}{2}\,\rho\,\vec{v}_x^{\,2})_J \, dR_1$$

$$N(2,1) = \sum_J \iiint_{SR_J} y\,(\tfrac{1}{2}\,\rho\,\vec{v}_x^{\,2})_J \, dR_1$$

(C-12b)

(Continued)

$$N(3,1) = \sum_J \iiint_{SR_J} z \left(\tfrac{1}{2} \rho \vec{v}_x^{\,2}\right)_J dR_1$$

$$N(4,1) = \sum_J \iiint_{SR_J} yz \left(\tfrac{1}{2} \rho \vec{v}_x^{\,2}\right)_J dR_1$$

(C-12b cont.)

$$N(5,1) = \sum_J \iiint_{SR_J} y^2 \left(\tfrac{1}{2} \rho \vec{v}_x^{\,2}\right)_J dR_1$$

$$N(6,1) = \sum_J \iiint_{SR_J} z^2 \left(\tfrac{1}{2} \rho \vec{v}_x^{\,2}\right)_J dR_1$$

$\vec{j}$ Component:

$$N(1,2) = C(1,2)\,G(3,2) + C(2,2)\,G(11,2) + C(3,2)\,G(1,2) + C(4,2)\,G(7,2) + C(5,2)\,G(2,2) + C(6,2)\,G(6,2)$$

$$N(2,2) = C(1,2)\,G(4,2) + C(2,2)\,G(12,2) + C(3,2)\,G(2,2) + C(4,2)\,G(8,2) + C(5,2)\,G(3,2) + C(6,2)\,G(7,2)$$

$$N(3,2) = C(1,2)\,G(8,2) + C(2,2)\,G(16,2) + C(3,2)\,G(6,2) + C(4,2)\,G(12,2) + C(5,2)\,G(7,2) + C(7,2)\,G(11,2)$$

(C-13a)

$$N(4,2) = C(1,2)\,G(14,2) + C(2,2)\,G(17,2) + C(3,2)\,G(7,2) + C(4,2)\,G(13,2) + C(5,2)\,G(8,2) + C(7,2)\,G(12,2)$$

$$N(5,2) = C(1,2)\,G(5,2) + C(2,2)\,G(13,2) + C(3,2)\,G(3,2) + C(4,2)\,G(9,2) + C(5,2)\,G(4,2) + C(7,2)\,G(8,2)$$

$$N(6,2) = C(1,2)\,G(13,2) + C(2,2)\,G(21,2) + C(3,2)\,G(11,2) + C(4,2)\,G(17,2) + C(5,2)\,G(12,2) + C(7,2)\,G(16,2)$$

where

$$N(1,2) = \sum_J \iiint_{SR_J} (\tfrac{1}{2} \rho \vec{v}_y^{\,2})_J \, dR_2$$

$$N(2,2) = \sum_J \iiint_{SR_J} z \, (\tfrac{1}{2} \rho \vec{v}_y^{\,2})_J \, dR_2$$

$$N(3,2) = \sum_J \iiint_{SR_J} x \, (\tfrac{1}{2} \rho \vec{v}_y^{\,2})_J \, dR_2 \qquad \text{(C-13b)}$$

$$N(4,2) = \sum_J \iiint_{SR_J} zx \, (\tfrac{1}{2} \rho \vec{v}_y^{\,2})_J \, dR_2$$

$$N(5,2) = \sum_J \iiint_{SR_J} z^2 \, (\tfrac{1}{2} \rho \vec{v}_y^{\,2})_J \, dR_2$$

$$N(6,2) = \sum_J \iiint_{SR_J} x^2 \, (\tfrac{1}{2} \rho \vec{v}_y^{\,2})_J \, dR_2$$

and $dR_2 = dy\ dz\ dx$.

$\vec{k}$ Component:

$$\begin{aligned} N(1,3) &= C(1,3)\ G(3,3) + C(2,3)\ G(11,3) + C(3,3)\ G(1,3) \\ &\quad + C(4,3)\ G(7,3) + C(5,3)\ G(2,3) + C(6,3)\ G(6,3) \end{aligned}$$

$$\begin{aligned} N(2,3) &= C(1,3)\ G(4,3) + C(2,3)\ G(12,3) + C(3,3)\ G(2,3) \\ &\quad + C(4,3)\ G(8,3) + C(5,3)\ G(3,3) + C(6,3)\ G(7,3) \end{aligned}$$

$$\begin{aligned} N(3,3) &= C(1,3)\ G(8,3) + C(2,3)\ G(16,3) + C(3,3)\ G(6,3) \\ &\quad + C(4,3)\ G(12,3) + C(5,3)\ G(7,3) + C(6,3)\ G(11,3) \end{aligned} \qquad \text{(C-14a)}$$

$$\begin{aligned} N(4,3) &= C(1,3)\ G(14,3) + C(2,3)\ G(17,3) + C(3,3)\ G(7,3) \\ &\quad + C(4,3)\ G(13,3) + C(5,3)\ G(8,3) + C(6,3)\ G(12,3) \end{aligned}$$

$$\begin{aligned} N(5,3) &= C(1,3)\ G(5,3) + C(2,3)\ G(13,3) + C(3,3)\ G(3,3) \\ &\quad + C(4,3)\ G(9,3) + C(5.3)\ G(4,3) + C(6,3)\ G(8,3) \end{aligned}$$

(Continued)

$$N(6,3) = C(1,3)\ G(13,3) + C(2,3)\ G(21,3) + C(3,3)\ G(11,3) + C(4,3)\ G(17,3) + C(5,3)\ G(12,3) + C(6,3)\ G(16,3) \quad \text{(C-14a Cont.)}$$

where

$$N(1.3) = \sum_J \iiint_{SR_J} (\tfrac{1}{2}\ \rho\ \vec{v}_z^{\,2})\ dR_3$$

$$N(2,3) = \sum_J \iiint_{SR_J} x\ (\tfrac{1}{2}\ \rho\ \vec{v}_z^{\,2})\ dR_3$$

$$N(3,3) = \sum_J \iiint_{SR_J} y\ (\tfrac{1}{2}\ \rho\ \vec{v}_z^{\,2})\ dR_3 \qquad \text{(C-14b)}$$

$$N(4,3) = \sum_J \iiint_{SR_J} xy\ (\tfrac{1}{2}\ \rho\ \vec{v}_z^{\,2})\ dR_3$$

$$N(5,3) = \sum_J \iiint_{SR_J} x^2\ (\tfrac{1}{2}\ \rho\ \vec{v}_z^{\,2})\ dR_3$$

$$N(6,3) = \sum_J \iiint_{SR_J} y^2\ (\tfrac{1}{2}\ \rho\ \vec{v}_z^{\,2})\ dR_3\ .$$

The relationships between the coefficients of the momentum expressions and the kinetic energy expressions are listed in Table C-2.

Table C-2. Relationships Between The Coefficients of Distributions at $t_s + \Delta t$

The Density Coefficient

A'

$\vec{i}$ Component	$\vec{j}$ Component	$\vec{k}$ Component

The Velocity Coefficients

A(1,1)	A(1,2)	A(1,3)
A(2,1)	A(2,2)	A(2,3)
A(3,1)	A(3,2)	A(3,3)

The Momentum Coefficients

$B(1,1) = A'A(1,1)$	$B(1,2) = A'A(1,2)$	$B(1,3) = A'A(1,3)$
$B(2,1) = A'A(2,1)$	$B(2,2) = A'A(2,2)$	$B(2,3) = A'A(2,3)$
$B(3,1) = A'A(3,1)$	$B(3,2) = A'A(3,2)$	$B(3,3) = A'A(3,3)$

The Kinetic Energy Coefficients

$C(1,1) = 1/2\ A'A(1,1)^2$	$C(1,2) = 1/2\ A'A(1,2)^2$	$C(1,3) = 1/2\ A'A(1,3)^2$
$C(2,1) = 1/2\ A'A(2,1)^2$	$C(2,2) = 1/2\ A'A(2,2)^2$	$C(2,3) = 1/2\ A'A(2,3)^2$
$C(3,1) = 1/2\ A'A(3,1)^2$	$C(3,2) = 1/2\ A'A(3,2)^2$	$C(3,3) = 1/2\ A'A(3,3)^2$
$C(4,1) = A'A(1,1)A(3,1)$	$C(4,2) = A'A(1,2)A(2,2)$	$C(4,3) = A'A(1,3)A(2,3)$
$C(5,1) = A'A(1,1)A(3,1)$	$C(5,2) = A'A(1,2)A(3,2)$	$C(5,3) = A'A(1,3)A(3,3)$
$C(6,1) = A'A(2,1)A(3,1)$	$C(6,2) = A'A(2.2)A(3.2)$	$C(6,3) = A'A(2,3)A(3,3)$

LIST OF SYMBOLS

A'	- a constant density distribution.
$A(i,j)$	- coefficients for velocity distribution at $t_s + \Delta t$.
a_1**	- the average slope of $\vec{v}$ across three adjacent cells; a least square cubic fit.
$a_1, a_2, \ldots, a_4$	- coefficients for velocity distributions.
$B(i,j)$	- coefficients for momentum distributions.
b_1, b_2, and b_3	- coefficients for distribution of arbitrary parameter α.
$C(i,j)$	- coefficients for Kinetic Energy distribution at $t_s + \Delta t$.
c_1, c_2, and c_3	- coefficients of least square cubic fit of a_1 of adjacent cells.
dA	= dx dy.
dx, dy, dz	- fixed coordinate derivatives.
dR_1, dR_2, dR_3	- equals dx dy dz, dy dz dx, and dz dx dy respectively.
dR	- derivatives over volumes.
dR^*	- derivatives over surfaces.
D/Dt	- substantial derivative.
E^T	- total energy.
E^I	- internal energy.
E^K	- kinetic energy.
f	- function to be weighted.
f_i	- external force on species i.
$G_1, G_2, \ldots, G_6$	- Geometric Moments.
$G(i,j)$	- Geometric Moments.
I	- consecutive numbering of computational cells.
I_{max}	- maximum number of computational cells.

LIST OF SYMBOLS

$\vec{i}$	- unit directional vector.
$\vec{j}$	- unit directional vector.
$\vec{k}$	- unit directional vector.
k_1, k_2, k_3	- exponents for function f.
M(i,j)	- moments for momentum.
m_i	- mass of i^{th} species.
N(i,j)	- moments for kinetic energy.
P	- pressure.
$\vec{q}$	- energy flux.
S	- denotes columns of cells in fixed coordinates.
S1, S2,....,S7	- identifies parts of flowchart.
$SR(t_s)$	- limits of subregions at t_s.
$SR(t_s + \Delta t)$	- limits of subregions at $t_s + \Delta t$.
T	- denotes rows of cells in fixed coordinates.
t	- time.
Δt	- time step.
t_s	- an instant of time corresponding to start of cycle of computation.
t_0	- an instant of time corresponding to start of problem.
TC	- implies integration over total cell.
U	- an arbitrary function.
V	- an arbitrary function.
$\vec{v}$	- mass average velocity.
$\vec{v}_i$	- species velocity.

LIST OF SYMBOLS

$\vec{v}_x$, $\vec{v}_y$, $\vec{v}_z$	- velocity components.
w_i	- mass rate of production of the i^{th} species through chemical reactions.
x, y, z	- coordinates in fixed coordinate system.
∇	- the del operator; $\vec{i}\ \partial/\partial x + \vec{j}\ \partial/\partial y + \vec{k}\ \partial/\partial z$.
$\alpha/\partial t$	- partial derivative with respect to time.
μ	- fluid viscosity.
α	- an arbitrary physical parameter.
Δ	- delta.
ρ	- density distribution.
$\vec{\vec{\tau}}$	- stress tensor.

SUBSCRIPTS

i	- species
I	- cells in computational grid
J	- denotes SR's which are summed in a fixed I cell at $t_s + \Delta t$
K	- denotes SR's of Lagrangian cell at t_s
K_{max}	- maximum number of subregions of Lagrangian cell at t_s
S	- denotes subregions in Section III
s	- denotes time at start of cycle of computation
T	- denotes subregions in Section III
0	- denotes instant of time corresponding to the start of problem

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